Catalytic Enantioselective Cross-Couplings of Secondary Alkyl Electrophiles with Secondary Alkylmetal Nucleophiles: Negishi Reactions of Racemic Benzylic Bromides with Achiral Alkylzinc Reagents

Jörg T. Binder,[†] Christopher J. Cordier,[†‡] and Gregory C. Fu[†‡]*

[†]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States
[‡]Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125, United States

Supporting Information

Table of Contents

I. General Information

The following compounds were purchased and used as received: *tert*-leucine (R and S; Aldrich), isoquinoline-1-carbonitrile (Alfa Aesar), $NiBr_2$·glyme (Aldrich), CsI (Strem; anhydrous, 99.999%; beads), MgI_2 (Aldrich; anhydrous, 99.998%; beads), CH_2Cl_2 (Aldrich; anhydrous, 99.8%), and 1,4-dioxane (Aldrich; anhydrous, 99.8%).

HPLC analyses were carried out on an Agilent 1100 Series system with Daicel CHIRALCEL® and CHIRALPAK® columns (internal diameter 4.6 mm, column length 250 mm, particle size 5 μ).

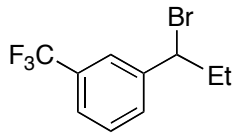
GC analyses were performed on a Hewlett Packard HP 6850 Series system with a Varian GC capillary column (WCOT fused silica 25 m × 0.25 mm; stationary phase: CP CHIRASIL-DEX CB; film thickness 0.25 μm).

II. Preparation of Electrophiles

The procedures and yields have not been optimized.

Bromination Procedure. A dry 100 mL round-bottom flask was charged with the benzylic alcohol (36 mmol) and then placed under a nitrogen atmosphere. Dry CH_2Cl_2 (18 mL) was

added, and the resulting solution was cooled to 0 °C. A solution of PBr_3 (7.0 g, 26 mmol, 0.72 equiv) in dry CH_2Cl_2 (18 mL) was added by syringe over a period of 5 min to the solution of the alcohol. The mixture was allowed to stir at 0 °C for 2 h. Next, water (20 mL) was added cautiously, and stirring was continued for another 5 min. Then, the mixture was transferred to a separatory funnel, and the organic layer was washed with 5% aqueous K_2CO_3 (50 mL). The aqueous layer was extracted with CH_2Cl_2 (50 mL), and the combined organic layers were washed with brine (50 mL), dried (Na_2SO_4), and concentrated under vacuum to give either a colorless or a yellow residue. This residue was taken up in Et_2O (10 mL), passed through an Acrodisc®, and concentrated to furnish the desired benzylic bromide as either a colorless or a yellow oil. The product was either purified by distillation or used without further purification.

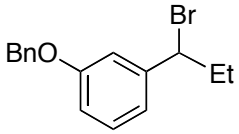


1-(1-Bromopropyl)-3-(trifluoromethyl)benzene. The title compound was prepared according to the Bromination Procedure, using 1-(3-(trifluoromethyl)phenyl)propan-1-ol (5.05 g, 24.7 mmol) and PBr_3 (4.82 g, 17.8 mmol). After distillation of the product, the compound was obtained as a colorless oil (2.03 g, 31%).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.63 (br s, 1 H), 7.61-7.53 (m, 2 H), 7.50-7.44 (m, 1 H), 4.88 (dd, *J* = 8.2, 6.7 Hz, 1 H), 2.36-2.24 (m, 1 H), 2.22-2.10 (m, 1 H), 1.02 (t, *J* = 7.3 Hz, 3 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.3, 131.2 (q, *J* = 32.6 Hz), 130.9, 129.4, 125.2 (q, *J* = 3.7 Hz), 124.3 (q, *J* = 3.7 Hz), 124.1 (q, *J* = 272.8 Hz), 55.8, 33.3, 13.0;

FT-IR (film): 2975, 2939, 2879, 1452, 1332, 1202, 1167, 1128, 1074, 900, 795, 700 cm^{-1}.

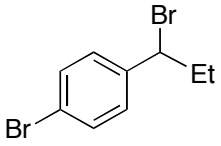


1-(Benzyloxy)-3-(1-bromopropyl)benzene. The title compound was prepared according to the Bromination Procedure, using 1-(3-(benzyloxy)phenyl)propan-1-ol (3.78 g, 12.4 mmol) and PBr_3 (2.41 g, 8.91 mmol). The product was obtained as a yellow oil (1.95 g, 52%) and was used without further purification.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47-7.42 (m, 2 H), 7.42-7.37 (m, 2 H), 7.36-7.31 (m, 1 H), 7.28-7.22 (m, 1 H), 7.05-6.97 (m, 2 H), 6.92-6.87 (m, 1 H), 5.07 (s, 2 H), 4.84 (app t, *J* = 7.4 Hz, 1 H), 2.34-2.21 (m, 1 H), 2.21-2.01 (m, 1 H), 0.99 (t, *J* = 7.3 Hz, 3 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.0, 143.8, 136.9, 129.8, 128.8, 128.2, 127.7, 120.1, 114.7, 114.2, 70.2, 57.5, 33.4, 13.1;

FT-IR (film): 3032, 2968, 1789, 1584, 1449, 1380, 1262, 1158, 1027, 836, 779, 736, 696 cm^{-1}.



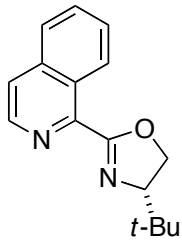
1-Bromo-4-(1-bromopropyl)benzene. The title compound was prepared according to the Bromination Procedure, using 1-(4-bromophenyl)propan-1-ol (2.59 g, 9.30 mmol) and PBr_3 (1.81 g, 6.70 mmol). The product was obtained as a yellow oil (1.65 g, 82%) and was used without further purification.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49-7.45 (m, 2 H), 7.28-7.24 (m, 2 H), 4.85-4.79 (m, 1 H), 2.33-2.20 (m, 1 H), 2.19-2.07 (m, 1 H), 0.99 (t, J = 7.3 Hz, 3 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.3, 131.9, 129.1, 122.2, 56.3, 33.3, 13.0;

FT-IR (film): 2969, 2934, 2875, 1489, 1457, 1406, 1074, 1011, 820, 795, 722 cm^{-1}.

III. Preparation of Ligand 1



(*S*)-4-(*tert*-Butyl)-2-(isoquinolin-1-yl)-4,5-dihydrooxazole (1). In a 250 mL flask, $ZnCl_2$ (526 mg, 3.86 mmol) was melted under high vacuum and cooled under argon. Chlorobenzene (140 mL) was added, followed by isoquinoline-1-carbonitrile (2.95 g, 19.1 mmol) and (*S*)-*tert*-leucinol[1] (2.92 g, 24.9 mmol). The resulting mixture was heated at 140 °C for 48 h. Next, the mixture was allowed to cool to r.t., and it was concentrated under reduced pressure. The residue was dissolved in CH_2Cl_2 (100 mL), and the resulting solution was transferred to a separatory funnel and washed with water (200 mL). The aqueous layer was extracted with CH_2Cl_2 (3 × 100 mL), and the combined organic layers were washed with brine, dried (Na_2SO_4), and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (using a hexanes–ethyl acetate gradient, 90:10 → 60:40). Recrystallization of the white solid from a hexane–CH_2Cl_2 mixture (40:1) yielded the product as colorless needles (2.46 g, 51%).

$[\alpha]^{24}_D$ = –84.4 (c = 1.0, $CHCl_3$);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.34-9.30 (m, 1 H), 8.63 (d, J = 5.6 Hz, 1 H), 7.88-7.85 (m, 1 H), 7.78-7.75 (m, 1 H), 7.75-7.66 (m, 2 H), 4.55-4.46 (m, 1 H), 4.37-4.28 (m, 2 H), 1.07 (s, 9 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.9, 146.5, 141.9, 136.8, 130.4, 128.6, 127.6, 127.5, 127.2, 123.4, 77.7, 68.3, 34.2, 26.2;

FT-IR (film): 3054, 2957, 2869, 1653, 1617, 1558, 1363, 1132, 1003, 832, 754, 669 cm^{-1};

LR-MS (ESI) calcd for $C_{16}H_{19}N_2O$ ($M+H^+$): 255.2, found: 255.2.

(1) Prepared according to: Krout, M. R.; Mohr, J. T.; Stoltz, B. M. *Org. Synth.* **2009**, *86*, 181–193.

IV. Asymmetric Secondary–Secondary Negishi Cross-Couplings

General procedure for the preparation of alkylzinc solutions (~1.0 M). A 20 mL vial was charged with zinc powder (980 mg, 15 mmol, 1.5 equiv), closed with a septum cap, and heated at 80 °C under high vacuum for 30 min. After backfilling the vial with nitrogen, 1,4-dioxane was added (to a total volume of 10 mL) by syringe. The septum cap was removed, iodine (130 mg, 0.51 mmol, 0.050 equiv) was added, and the vial was flushed with nitrogen. After the red color of iodine had faded (~30 min), the alkyl iodide[2] (10 mmol) was added. The colorless reaction mixture was stirred vigorously at r.t. for 14 h (the disappearance of the alkyl iodide and the formation of the alkylzinc reagent can readily be monitored by ^{1}H NMR spectroscopy). The gray mixture (~1.0 M) was filtered in a glove box through an Acrodisc® to give a colorless to slightly yellow solution, which can be stored at r.t. under an inert atmosphere for several days or in a glove box freezer at –35 °C for several weeks. The alkylzinc solution was often titrated by the Knochel method for organozinc titration, using iodine,[3] which routinely established that the alkylzinc reagent had been formed in good yield (final concentration: 0.95 to 1.0 M).

Preparation of a catalyst–ligand stock solution. In a glove box, an oven-dried 20 mL vial equipped with a stir bar was charged with $NiBr_2$·glyme (34.0 mg, 0.110 mmol). A solution of ligand (*S*)-**1** (36.4 mg, 0.143 mmol) in CH_2Cl_2 (4.4 mL), prepared in a separate vial, was added to the 20 mL vial that contained $NiBr_2$·glyme. The vial was capped, and the resulting suspension was stirred at r.t. for 10 min, at which time it had turned dark orange. Stirring was continued for an additional 30 min.

General Procedure 1: Cross-coupling of cyclopentylzinc iodide with acyclic benzylic bromides (Table 2, entries 1–11; for a glove box-free procedure, see below). In a glove box, an oven-dried 20 mL vial equipped with a stir bar was charged with finely ground CsI (301 mg, 1.16 mmol) and CH_2Cl_2 (2.0 mL). The catalyst–ligand stock solution (4.0 mL; 0.10 mmol of $NiBr_2$·glyme, 0.13 mmol of (*S*)-**1**) was added, and the resulting mixture was stirred for 2 min. A solution of the benzylic bromide (1.00 mmol) in CH_2Cl_2 (1.0 mL), prepared in a 4 mL vial, was transferred by pipette to the reaction vial. The 4 mL vial was rinsed with CH_2Cl_2 (0.5 mL x2), and the washings were transferred to the reaction vial. The reaction vial was closed with a septum cap, the septum seal was wrapped with electrical tape, and the reaction mixture was stirred for 2 min. Next, the vial was taken out of the glove box and then cooled to –30 °C. To the vigorously stirred solution was added cyclopentylzinc iodide (1.8 mL of an ~1.0 M solution in 1,4-dioxane; 1.8 mmol), in a continuous flow over 10 seconds, with two 1 mL syringes (both charged with 0.9 mL of the nucleophile solution inside the glove box). During this time, the reaction mixture turned from dark orange to very dark red or black. The septum cap was sealed using grease, and the mixture was stirred vigorously at –30 °C for 30–48 h. Then, the reaction was quenched by the addition of EtOH (1 mL), and the mixture was allowed to warm to r.t. Next, it was filtered through an Acrodisc®. The filtrate was concentrated under vacuum to a volume of approximately 1 mL, and the residue was purified by preparative TLC on silica to furnish the desired product.

A second run was performed with (*R*)-**1**.

---

(2) Prepared according to: Smith, S. W.; Fu, G. C. *Angew. Chem., Int. Ed.* **2008**, *47*, 9334–9336.

(3) Krasovskiy, A.; Knochel, P. *Synthesis* **2006**, 890–891.

Glove box-free procedure: A 20 mL vial was charged with zinc powder (980 mg, 15 mmol, 1.5 equiv), closed with a septum cap, and heated to 80 °C under high vacuum for 30 min. After back-filling the vial with nitrogen, 1,4-dioxane added (to a total volume of 10 mL) by syringe. The septum cap was removed, iodine (130 mg, 0.51 mmol, 0.050 equiv) was added, and the vial was flushed with nitrogen. After the red color of iodine had faded (~30 min), the alkyl iodide (10 mmol) was added. The colorless reaction mixture was stirred vigorously at r.t. for 14 h. The gray mixture (~1.0 M) was allowed to settle without stirring for 1 h, and then it was filtered by cannula into a separate 20 mL vial under nitrogen.

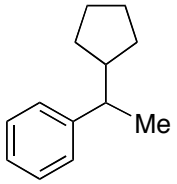
Preparation of a catalyst–ligand stock solution. In air, an oven-dried 20 mL vial equipped with a stir bar was charged $NiBr_2$·glyme (34.0 mg, 0.110 mmol), and a 4 mL vial was charged with ligand (*S*)-**1** (36.4 mg, 0.143 mmol). The vials were evacuated and back-filled with nitrogen three times. CH_2Cl_2 (3.0 mL) was added to the 4 mL vial, and this solution of ligand (*S*)-**1** was added by syringe to the 20 mL vial that contained $NiBr_2$·glyme. Additional CH_2Cl_2 (1.4 mL) was used to rinse the 4 mL vial, and this was transferred by syringe to the 20 mL vial. The resulting suspension was stirred under nitrogen at r.t. for 10 min, at which time it had turned dark orange. Stirring was continued for an additional 30 min.

Cross-coupling procedure. In air, an oven-dried 20 mL vial equipped with a stir bar was charged with finely ground CsI (301 mg, 1.16 mmol) and then evacuated and back-filled with nitrogen three times. Next, CH_2Cl_2 (2.0 mL) was added, yielding a suspension. The catalyst–ligand stock solution (4.0 mL; 0.10 mmol of $NiBr_2$·glyme, 0.13 mmol of (*S*)-**1**) was added via syringe, and the resulting mixture was allowed to stir for 2 min. An oven-dried 4 mL vial was charged with the benzylic bromide (1.00 mmol) in air and then purged with nitrogen for 5 min. CH_2Cl_2 (1.0 mL) was added, and the resulting solution was transferred to the reaction vial via syringe. The 4 mL vial was rinsed with CH_2Cl_2 (0.5 mL x2), and the washings were transferred to the reaction vial. The reaction vial was closed with a septum cap, the septum seal was wrapped with electrical tape, and the reaction mixture was stirred for 2 min. Next, the vial was cooled to –30 °C, and then cyclopentylzinc iodide (1.8 mL of a ~1.0 M solution in 1,4-dioxane; 1.8 mmol) was added slowly, in a continuous flow, with two 1 mL syringes (both charged with 0.9 mL of the nucleophile solution) over a period of 10 sec to the vigorously stirred solution. During this time, the reaction mixture turned from dark orange to very dark red or black. The septum cap was sealed using grease, and the mixture was stirred vigorously at –30 °C for 30–48 h. Then, the reaction was quenched by the addition of EtOH (1 mL), and the mixture was allowed to warm to r.t. Next, it was filtered through an Acrodisc®. The filtrate was concentrated under vacuum to a volume of approximately 1 mL, and the residue was purified by preparative TLC on silica to furnish the desired product.

(1-Cyclopentylethyl)benzene. This compound was prepared according to the glove box-free procedure, using (±)-(1-bromoethyl)benzene (185 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction mixture was stirred at –30 °C for 40 h (both runs). After purification of the crude residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 156 mg (90%, 90% ee); 2nd run: 166 mg (95%, 92% ee).

NMR spectral data were identical to material prepared according to General Procedure 1 (Table 2, entry 1).



(1-Cyclopentylethyl)benzene (Table 2, entry 1). The title compound was prepared according to General Procedure 1, using (±)-(1-bromoethyl)benzene (185 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction mixture was stirred at –30 °C for 45 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 162 mg (93%, 94% ee); 2nd run: 154 mg (88%, 95% ee).

The ee was determined by GC analysis (75→150 °C, ramp: 1 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 36.76 min, t_r (minor): 37.61 min.

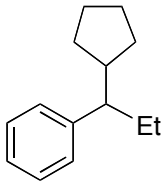
$[\alpha]^{24}_D$ = +22.0 (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.31-7.25 (m, 2 H), 7.21-7.15 (m, 3 H), 2.48-2.38 (m, 1 H), 2.02-1.86 (m, 2 H), 1.72-1.60 (m, 1 H), 1.60-1.49 (m, 2 H), 1.49-1.33 (m, 2 H), 1.30-1.16 (m, 4 H), 1.08-0.95 (m, 1 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.2, 128.2, 127.4, 125.8, 47.7, 46.3, 31.9, 31.6, 25.5, 25.2, 21.6;

FT-IR (film): 3026, 2955, 2870, 1492, 1451, 1374, 760, 699 cm^{-1};

GC-MS (EI) calcd for $C_{13}H_{18}$ (M^+): 174, found: 174.



(1-Cyclopentylpropyl)benzene (Table 2, entry 2). The title compound was prepared according to General Procedure 1, using (±)-(1-bromopropyl)benzene (199 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 31 h (1st run) and 42 h (2nd run). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 163 mg (87%, 91% ee); 2nd run: 152 mg (81%, 94% ee).

The ee was determined by GC analysis (75→150 °C, ramp: 1 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 41.07 min, t_r (minor): 41.85 min.

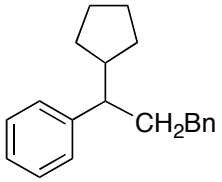
$[\alpha]^{24}_D$ = –2.2 (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30-7.25 (m, 2 H), 7.20-7.17 (m, 1 H), 7.16-7.12 (m, 2 H), 2.17 (td, *J* = 10.1, 3.6 Hz, 1 H), 2.07-1.89 (m, 2 H), 1.88-1.78 (m, 1 H), 1.70-1.60 (m, 1 H), 1.60-1.47 (m, 3 H), 1.46-1.29 (m, 2 H), 1.28-1.16 (m, 1 H), 1.02-0.91 (m, 1 H), 0.69 (t, *J* = 7.4 Hz, 3 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.7, 128.2, 128.0, 125.6, 54.2, 46.5, 31.8, 31.6, 28.1, 25.3, 24.9, 12.2;

FT-IR (film): 3062, 3027, 2956, 2870, 1653, 1559, 1452, 760, 700, 668 cm^{-1};

GC-MS (EI) calcd for $C_{14}H_{20}$ (M^+): 188, found: 188.



(1-Cyclopentylpropane-1,3-diyl)dibenzene (Table 2, entry 3). The title compound was prepared according to General Procedure 1, using (±)-(1-bromopropane-1,3-diyl)dibenzene (275 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 46 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 193 mg (73%, 96% ee); 2nd run: 186 mg (70%, 94% ee).

The ee was determined by HPLC analysis, using an OJ-H column; solvent system: 100% hexanes; flow rate: 1.0 mL/min; retention times for compound obtained using (*S*)-**1**: 9.96 min (major), 13.52 min (minor).

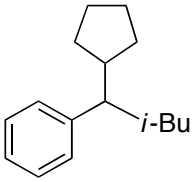
$[\alpha]^{24}_{D} = -20.0$ (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.35-7.30 (m, 2 H), 7.29-7.22 (m, 3 H), 7.21-7.15 (m, 3 H), 7.13-7.09 (m, 2 H), 2.48-2.39 (m, 1 H), 2.38-2.27 (m, 2 H), 2.18-2.09 (m, 1 H), 2.08-1.98 (m, 1 H), 1.98-1.85 (m, 2 H), 1.69-1.47 (m, 3 H), 1.46-1.27 (m, 2 H), 1.25-1.14 (m, 1 H), 1.04-0.92 (m, 1 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.5, 142.9, 128.5, 128.3 (3C), 126.0, 125.7, 52.0, 46.9, 37.2, 34.0, 31.9, 31.7, 25.4, 25.0;

FT-IR (film): 3083, 3061, 3026, 2949, 2866, 1602, 1495, 1452, 763, 748, 699 cm^{-1};

GC-MS (EI) calcd for $C_{20}H_{24}$ (M^+): 264, found: 264.



(1-Cyclopentyl-3-methylbutyl)benzene (Table 2, entry 4). The title compound was prepared according to General Procedure 1, using (±)-(1-bromo-3-methylbutyl)benzene (227 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 48 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 170 mg (79%, 94% ee); 2nd run: 153 mg (71%, 92% ee).

The ee was determined by GC analysis (75→150 °C, ramp: 1 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (minor): 48.89 min, t_r (major): 49.22 min.

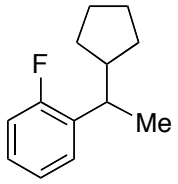
$[\alpha]^{24}_{D} = -26.8$ (*c* = 1.0, $CDCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30-7.24 (m, 2 H), 7.20-7.12 (m, 3 H), 2.39-2.30 (m, 1 H), 1.99-1.86 (m, 2 H), 1.70-1.45 (m, 5 H), 1.45-1.33 (m, 1 H), 1.33-1.12 (m, 3 H), 1.02-0.91 (m, 1 H), 0.83 (d, *J* = 6.5 Hz, 3 H), 0.79 (d, *J* = 6.6 Hz, 3 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.1, 128.2, 128.1, 125.7, 50.0, 47.5, 44.8, 31.9, 31.8, 25.4 (2 C), 25.0, 24.4, 21.3;

FT-IR (film): 3062, 3026, 2954, 2867, 1653, 1540, 1466, 1451, 1383, 1367, 700 cm^{-1};

GC-MS (EI) calcd for $C_{16}H_{24}$ (M^+): 216, found: 216.



1-(1-Cyclopentylethyl)-2-fluorobenzene (Table 2, entry 5). The title compound was prepared according to General Procedure 1, using (±)-1-(1-bromoethyl)-2-fluorobenzene (203 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). Note that the cross-coupling of this substrate was found to be particularly reliant on the CsI being finely ground. The reaction was stirred at –30 °C for 48 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 93 mg (48%, 85% ee); 2nd run: 92 mg (48%, 88% ee).

The ee was determined by GC analysis (75→150 °C, ramp: 1 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 34.19 min, t_r (minor): 35.08 min.

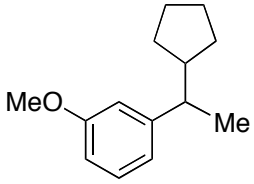
$[\alpha]^{24}_D$ = –28.7 (*c* = 1.0, $CHCl_3$; for compound obtained using (*R*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.22 (td, *J* = 7.4, 1.9 Hz, 1 H), 7.17-7.10 (m, 1 H), 7.09-7.05 (m, 1 H), 7.02-6.96 (m, 1 H), 2.88-2.79 (m, 1 H), 2.10-1.97 (m, 1 H), 1.96-1.87 (m, 1 H), 1.73-1.38 (m, 5 H), 1.31-1.18 (m, 4 H), 1.12-0.98 (m, 1 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.8 (d, *J* = 243.8 Hz), 134.5, 128.6 (d, *J* = 5.1 Hz), 127.0 (d, *J* = 8.3 Hz), 124.1 (d, *J* = 3.6 Hz), 115.3 (d, *J* = 11.8 Hz), 46.7, 38.6 (d, *J* = 1.2 Hz), 31.7, 31.6, 25.5, 25.2, 20.4;

FT-IR (film): 2955, 2870, 1490, 1451, 1228, 754 cm^{-1};

GC-MS (EI) calcd for $C_{13}H_{17}F$ (M^+): 192, found: 192.



1-(1-Cyclopentylethyl)-3-methoxybenzene (Table 2, entry 6). The title compound was prepared according to General Procedure 1, using (±)-1-(1-bromoethyl)-3-methoxybenzene (215 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 42 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 173 mg (85%, 95% ee); 2nd run: 179 mg (87%, 94% ee).

The ee was determined by HPLC analysis, using an AD-H column; solvent system: 100% hexanes; flow rate: 1.0 mL/min; retention times for compound obtained using (*S*)-**1**: 6.90 min (minor), 8.22 min (major).

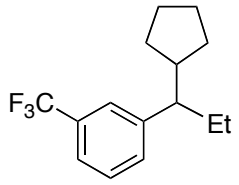
$[\alpha]^{24}_D$ = +26.4 (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.21 (t, *J* = 7.7 Hz, 1 H), 6.80 (dt, *J* = 7.7, 1.1 Hz, 1 H), 6.77-6.72 (m, 2 H), 3.82 (s, 3 H), 2.46-2.37 (m, 1 H), 2.02-1.86 (m, 2 H), 1.73-1.62 (m, 1 H), 1.62-1.51 (m, 2 H), 1.51-1.38 (m, 2 H), 1.30-1.17 (m, 4 H), 1.11-0.98 (m, 1 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.5, 149.8, 129.1, 119.8, 113.3, 110.6, 55.1, 47.5, 46.3, 31.8, 31.5, 25.4, 25.1, 21.5;

FT-IR (film): 2955, 2870, 2834, 1789, 1601, 1584, 1487, 1285, 1263, 1154, 1046, 776, 701 cm^{-1};

GC-MS (EI) calcd for $C_{14}H_{20}$ (M^+): 204, found: 204.



1-(1-Cyclopentylpropyl)-3-(trifluoromethyl)benzene (Table 2, entry 7). The title compound was prepared according to General Procedure 1, using (±)-1-(1-bromopropyl)-3-(trifluoromethyl)benzene (267 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 42 h (1st run) and 46 h (2nd run). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 134 mg (52%, 90% ee); 2nd run: 127 mg (50%, 92% ee).

The ee was determined by GC analysis (75→130 °C, ramp: 0.5 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 57.39 min, t_r (minor): 58.47 min.

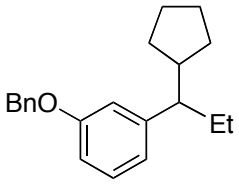
$[\alpha]^{24}_D$ = –2.8 (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.46-7.41 (m, 1 H), 7.41-7.35 (m, 2 H), 7.34-7.29 (m, 1 H), 2.24 (td, *J* = 10.4 Hz, *J* = 3.7 Hz, 1 H), 2.07-1.81 (m, 3 H), 1.71-1.47 (m, 4 H), 1.47-1.36 (m, 1 H), 1.35-1.25 (m, 1 H), 1.25-1.16 (m, 1 H), 0.98-0.87 (m, 1 H), 0.68 (t, *J* = 7.4 Hz, 3 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.8, 131.7, 130.6 (q, *J* = 31.9 Hz), 128.6, 124.9 (q, *J* = 3.7 Hz), 124.6 (q, *J* = 272.2 Hz), 122.8 (q, *J* = 3.6 Hz), 54.3, 46.5, 31.9, 31.7, 28.1, 25.4, 25.0, 12.2;

FT-IR (film): 2959, 2874, 1448, 1325, 1163, 1126, 1075, 802, 705, 659 cm^{-1};

GC-MS (EI) calcd for $C_{15}H_{19}F_3$ (M^+): 256, found: 256.



1-(Benzyloxy)-3-(1-cyclopentylpropyl)benzene (Table 2, entry 8). The title compound was prepared according to General Procedure 1, using (±)-1-(benzyloxy)-3-(1-bromopropyl)benzene (305 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 46 h (both runs). After purification of the residue by preparative TLC on silica (hexanes/ethylacetate 98:2), the title compound was isolated as a colorless oil.

1st run: 179 mg (61%, 90% ee); 2nd run: 199 mg (68%, 91% ee).

The ee was determined by HPLC analysis, using an OD-H column; solvent system: 100% hexanes; flow rate: 1.0 mL/min; retention times for compound obtained using (*S*)-**1**: 13.80 min (major), 15.13 min (minor).

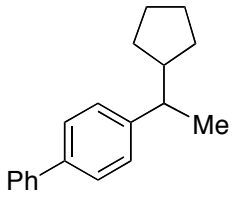
$[\alpha]^{24}_{D} = -0.7$ (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.48-7.44 (m, 2 H), 7.42-7.36 (m, 2 H), 7.35-7.30 (m, 1 H), 7.22-7.17 (m, 1 H), 6.83-6.73 (m, 3 H), 5.06 (s, 2 H), 2.14 (td, *J* = 10.3, 3.5 Hz, 1 H), 2.03-1.87 (m, 2 H), 1.87-1.76 (m, 1 H), 1.70-1.30 (m, 6 H), 1.26-1.13 (m, 1 H), 1.04-0.90 (m, 1 H), 0.70 (t, *J* = 7.4 Hz, 3 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.8, 147.6, 137.4, 129.0, 128.7, 128.0, 127.8, 121.2, 115.2, 111.7, 70.1, 54.4, 46.6, 31.9, 31.7, 28.1, 25.4, 25.0, 12.3;

FT-IR (film): 3033, 2954, 2869, 1583, 1486, 1448, 1379, 1291, 1259, 1154, 1027, 733, 696 cm^{-1};

GC-MS (EI) calcd for $C_{21}H_{26}O$ (M^+): 294, found: 294.



4-(1-Cyclopentylethyl)-1,1'-biphenyl (Table 2, entry 9). The title compound was prepared according to General Procedure 1, using (±)-4-(1-bromoethyl)-1,1'-biphenyl (261 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 46 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 199 mg (79%, 93% ee); 2nd run: 204 mg (81%, 96% ee).

The ee was determined by HPLC analysis, using an OJ-H column; solvent system: 100% hexanes; flow rate: 0.5 mL/min; retention times for compound obtained using (*S*)-**1**: 39.64 min (major), 44.06 min (minor).

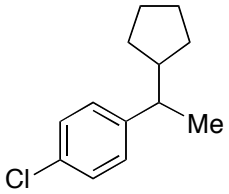
$[\alpha]^{24}_{D} = +33.5$ (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62-7.58 (m, 2 H), 7.55-7.50 (m, 2 H), 7.47-7.40 (m, 2 H), 7.36-7.30 (m, 1 H), 7.28-7.24 (m, 2 H), 2.54-2.44 (m, 1 H), 2.06-1.88 (m, 2 H), 1.74-1.63 (m, 1 H), 1.63-1.51 (m, 2 H), 1.51-1.40 (m, 2 H), 1.34-1.19 (m, 4 H), 1.14-1.00 (m, 1 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 147.3, 141.3, 138.7, 128.8, 127.8, 127.1, 127.0 (2 C), 47.7, 46.0, 32.0, 31.6, 25.5, 25.3, 21.6;

FT-IR (film): 3042, 2946, 2863, 1653, 1559, 1408, 1119, 834, 762, 726, 689 cm^{-1};

GC-MS (EI) calcd for $C_{19}H_{22}$ (M^+): 250, found: 250.



1-Chloro-4-(1-cyclopentylethyl)benzene (Table 2, entry 10). The title compound was prepared according to General Procedure 1, using (±)-1-(1-bromoethyl)-4-chlorobenzene (220 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred vigorously at –30 °C for 42 h (1st run) and 46 h (2nd run). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 157 mg (75%, 93% ee); 2nd run: 159 mg (76%, 93% ee).

This compound was also prepared on a 5.0 mmol scale, using (±)-1-(1-bromoethyl)-4-chlorobenzene (1.10 g, 5.00 mmol) and cyclopentylzinc iodide (~0.95 M in 1,4-dioxane; 9.5 mL, 9.0 mmol). The reaction was stirred vigorously at –30 °C for 48 h (both runs). After purification of the residue by flash chromatography on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 795 mg (76%, 92% ee); 2nd run: 741 mg (71%, 92% ee).

The ee was determined by GC analysis (75→150 °C, ramp: 1 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 59.59 min, t_r (minor): 60.77 min.

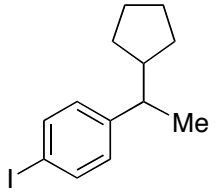
$[\alpha]^{24}_D$ = +25.5 (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.26-7.20 (m, 2 H), 7.12-7.07 (m, 2 H), 2.35-2.26 (m, 1 H), 1.97-1.83 (m, 2 H), 1.71-1.60 (m, 1 H), 1.60-1.49 (m, 2 H), 1.49-1.31 (m, 2 H), 1.29-1.14 (m, 4 H), 1.04-0.91 (m, 1 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.6, 131.3, 128.7, 128.4, 47.6, 45.7, 31.8, 31.5, 25.4, 25.2, 21.6;

FT-IR (film): 2956, 2870, 1653, 1492, 1410, 1374, 1095, 1014, 826, 720, 666 cm^{-1};

GC-MS (EI) calcd for $C_{13}H_{17}Cl$ (M^+): 208, found: 208.



1-Iodo-4-(1-cyclopentylethyl)benzene (Table 2, entry 11). The title compound was prepared according to General Procedure 1, using (±)-(1-bromoethyl)-4-iodobenzene (311 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.1 mL, 1.1 mmol; note: a smaller excess was used than in General Procedure 1, to decrease the possibility of coupling the aryl iodide). The reaction was stirred vigorously at –30 °C for 36 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 223 mg (74%, 91% ee); 2nd run: 221 mg (74%, 91% ee). Both runs employed (*S*)-**1**.

The ee was determined by GC analysis (75→170 °C, ramp: 1 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 83.53 min, t_r (minor): 84.69 min.

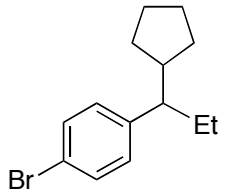
$[\alpha]^{25}_{D}$ =+21.51 (*c* = 1.0 $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62-7.54 (m, 2 H), 6.97-6.88 (m, 2 H), 2.37 (dq, *J* = 9.2, 6.9 Hz, 1 H), 1.98-1.81 (m, 2 H), 1.72-1.12 (m, 8 H), 1.05-0.81 (m, 2 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 147.7, 137.2, 129.5, 90.6, 47.4, 45.8, 31.7, 31.4, 25.3, 25.1, 21.3;

FT-IR (film): 3070, 3017, 2952, 2868, 1894, 1642, 1586, 1485, 1451, 1402, 1373, 1328, 1293, 1102, 1061, 1005, 938, 819, 778, 716;

LC-MS (ES) calcd for $C_{13}H_{17}I$ (M^+): 300, found 300.



1-Bromo-4-(1-cyclopentylpropyl)benzene (Table 2, entry 12). The title compound was prepared according to General Procedure 1, using (±)-1-bromo-4-(1-bromopropyl)benzene (278 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 42 h (1st run) and 45 h (2nd run). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 190 mg (71%, 91% ee); 2nd run: 171 mg (64%, 92% ee).

The ee was determined by GC analysis (75→150 °C, ramp: 1 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 72.28 min, t_r (minor): 72.99 min.

$[\alpha]^{24}_{D}$ = +1.2 (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.41-7.35 (m, 2 H), 7.03-6.97 (m, 2 H), 2.17-2.07 (m, 1 H), 2.01-1.86 (m, 2 H), 1.86-1.76 (m, 1 H), 1.69-1.58 (m, 1 H), 1.58-1.37 (m, 4 H), 1.36-1.25 (m, 1 H), 1.25-1.11 (m, 1 H), 0.97-0.85 (m, 1 H), 0.66 (t, *J* = 7.4 Hz, 3 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.8, 131.2, 120.0, 119.4, 53.8, 46.5, 31.9, 31.7, 28.1, 25.4, 25.0, 12.2;

FT-IR (film): 2955, 2870, 1653, 1559, 1488, 1457, 1405, 1074, 1010, 815, 668 cm^{-1};

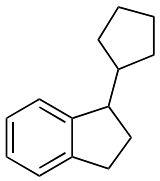
GC-MS (EI) calcd for $C_{14}H_{19}Br$ (M^+): 266, found: 266.

Preparation of a catalyst–ligand stock solution. In a glove box, an oven-dried 20 mL vial equipped with a stir bar was charged with $NiBr_2$·glyme (34.0 mg, 0.110 mmol), ligand (*S*)-**1** (36.4 mg, 0.143 mmol), and then CH_2Cl_2 (4.4 mL). The resulting suspension was stirred at r.t. for 10 min, at which time it had turned dark orange.

General Procedure 2: Cross-coupling of cyclopentylzinc iodide with cyclic benzylic bromides (Table 2, entries 12–14). In a glove box, an oven-dried 20 mL vial equipped with a stir bar was charged with finely ground MgI_2 (323 mg, 1.16 mmol) and CH_2Cl_2 (2.0 mL). The catalyst–ligand stock solution (4.0 mL; 0.10 mmol of $NiBr_2$·glyme, 0.13 mmol of (*S*)-**1**) was added by syringe, and the resulting mixture was stirred for 2 min. A solution of the benzylic bromide (1.00 mmol) in CH_2Cl_2 (1.0 mL), prepared in a 4 mL vial, was transferred by pipette to the reaction vial. The 4 mL vial was rinsed with CH_2Cl_2 (0.5 mL x2), and the washings were transferred to the reaction vial. The reaction vial was closed with a septum cap, the septum seal

was wrapped with electrical tape, and the reaction mixture was stirred for 2 min. Next, the vial was taken out of the glove box and then cooled to –30 °C. To the vigorously stirred solution was added cyclopentylzinc iodide (1.8 mL of an ~1.0 M solution in 1,4-dioxane; 1.8 mmol), in a continuous flow over 10 seconds, with two 1 mL syringes (both charged with 0.9 mL of the nucleophile solution inside the glove box). During this time, the reaction mixture turned from dark orange to very dark red or black. The septum cap was sealed using grease, and the mixture was stirred vigorously at –30 °C for 30–48 h. Then, the reaction was quenched by the addition of EtOH (1 mL), and the mixture was allowed to warm to r.t. Next, it was filtered through an Acrodisc®. The filtrate was concentrated under vacuum to a volume of approximately 1 mL, and the residue was purified by preparative TLC on silica to furnish the desired product.

A second run was performed with (*R*)-**1**.



1-Cyclopentyl-2,3-dihydro-1*H*-indene (Table 2, entry 13). The title compound was prepared according to General Procedure 2, using (±)-1-bromoindane (197 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 30 h (1st run) and 42 h (2nd run). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 130 mg (70%, 96% ee); 2nd run: 145 mg (78%, 96% ee).

The ee was determined by HPLC analysis, using an OJ-H column; solvent system: 100% hexanes; flow rate: 1.0 mL/min; retention times for compound obtained using (*S*)-**1**: 4.62 min (minor), 4.99 min (major).

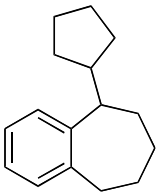
$[\alpha]^{24}_{D} = -11.5$ (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.29-7.24 (m, 1 H), 7.23-7.18 (m, 1 H), 7.16-7.11 (m, 2 H), 3.11-3.04 (m, 1 H), 2.97-2.88 (m, 1 H), 2.85-2.76 (m, 1 H), 2.23-2.13 (m, 1 H), 2.12-2.01 (m, 1 H), 1.93-1.80 (m, 2 H), 1.79-1.47 (m, 5 H), 1.44-1.32 (m, 1 H), 1.29-1.18 (m, 1 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 147.6, 144.5, 126.2, 125.9, 124.6, 124.5, 50.0, 44.5, 31.5, 31.4, 30.6, 30.4, 25.7, 25.3;

FT-IR (film): 2952, 2866, 1653, 1576, 1559, 1457, 749, 668 cm^{-1};

GC-MS (EI) calcd for $C_{14}H_{18}$ (M^+): 186, found: 186.



5-Cyclopentyl-6,7,8,9-tetrahydro-*5H*-benzocycloheptene (Table 2, entry 14). The title compound was prepared according to General Procedure 2, using (±)-5-bromo-6,7,8,9-tetrahydro-*5H*-benzocycloheptene (225 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 48 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the title compound was isolated as a colorless oil.

1st run: 165 mg (77%, 98% ee); 2nd run: 174 mg (81%, 97% ee).

The ee was determined by GC analysis (75→175 °C, ramp: 1 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 71.12 min, t_r (minor): 71.51 min.

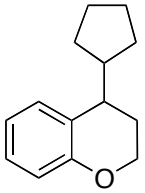
$[\alpha]^{25}_D$ = +7.0 (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.12-7.07 (m, 4 H), 2.97 (app t, *J* = 12.8 Hz, 1 H), 2.79 (dd, *J* = 14.1, 8.4 Hz, 1 H), 2.63-2.54 (m, 1 H), 2.45 (dquin, *J* = 9.8, 6.7 Hz, 1 H), 2.06-1.33 (m, 12 H), 1.37-1.31 (m, 1 H), 1.22-1.09 (m, 1 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.9, 142.1, 129.9 (2C), 125.6, 125.5, 52.5, 40.8, 36.4, 32.8, 31.5, 31.3, 28.3, 28.2, 25.4, 25.2;

FT-IR (film): 3058, 3014, 2918, 2856, 2689, 1490, 1447, 1369, 1312, 1060, 962, 938, 756, 746;

GC-MS (EI) cald for $C_{16}H_{22}$ (M^+): 214, found 214.



4-Cyclopentylchroman (Table 2, entry 15). The title compound was prepared according to General Procedure 2, using (±)-4-bromochroman (213 mg, 1.00 mmol) and cyclopentylzinc iodide (~1.0 M in 1,4-dioxane; 1.8 mL, 1.8 mmol). The reaction was stirred at –30 °C for 46 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the compound was subjected to another preparative TLC purification using reversed phase TLC plates (MeCN/H_2O 8:2) and isolated as a colorless oil.

1st run: 103 mg (51%, 94% ee); 2nd run: 114 mg (56%, 95% ee).

The ee was determined by GC analysis (75→150 °C, ramp: 1 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 71.76 min, t_r (minor): 73.19 min.

$[\alpha]^{24}_D$ = +1.6 (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.16-7.07 (m, 2 H), 6.85-6.77 (m, 2 H), 4.31-4.19 (m, 2 H), 2.69-2.61 (m, 1 H), 2.18-1.91 (m, 3 H), 1.84-1.63 (m, 4 H), 1.62-1.48 (m, 2 H), 1.48-1.36 (m, 1 H), 1.29-1.14 (m, 1 H);

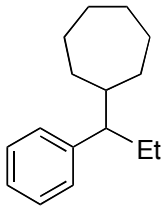
^{13}C NMR ($CDCl_3$, 100 MHz): δ 154.3, 129.9, 127.4, 126.3, 119.5, 116.6, 63.4, 44.9, 38.8, 31.8, 29.7, 25.7, 25.4, 24.7;

FT-IR (film): 2952, 2869, 1580, 1490, 1452, 1267, 1224, 1118, 1020, 752 cm^{-1};
GC-MS (EI) calcd for $C_{14}H_{18}O$ (M^+): 202, found: 202.

Preparation of a catalyst–ligand stock solution. In a glove box, an oven-dried 20 mL vial equipped with a stir bar was charged with $NiBr_2$·glyme (34.0 mg, 0.110 mmol), ligand (*S*)-**1** (36.4 mg, 0.143 mmol), and then CH_2Cl_2 (4.4 mL). The resulting suspension was stirred at r.t. for 10 min, at which time it had turned dark orange.

General Procedure 3: Cross-coupling of cycloheptylzinc iodide with acyclic benzylic bromides (Table 2, entries 15 and 16). In a glove box, an oven-dried 20 mL vial equipped with a stir bar was charged with finely ground CsI (301 mg, 1.16 mmol) and CH_2Cl_2 (2.0 mL). The catalyst–ligand stock solution (4.0 mL; 0.10 mmol of $NiBr_2$·glyme, 0.13 mmol of (*S*)-**1**) was added by syringe, and the resulting mixture was stirred for 2 min. A solution of the benzylic bromide (1.00 mmol) in CH_2Cl_2 (1.0 mL), prepared in a 4 mL vial, was transferred by pipette to the reaction vial. The 4 mL vial was rinsed with CH_2Cl_2 (0.5 mL x2), and the washings were transferred to the reaction vial. The reaction vial was closed with a septum cap, the septum seal was wrapped with electrical tape, and the reaction mixture was stirred for 2 min. Next, the vial was taken out of the glove box and then cooled to –30 °C. To the vigorously stirred solution was added cycloheptylzinc iodide (4.3 mL of an ~0.7 M solution in 1,4-dioxane; 3.0 mmol), in a continuous flow over 10 seconds, with two 1 mL syringes (both charged with 0.9 mL of the nucleophile solution inside the glove box). During this time, the reaction mixture turned from dark orange to very dark red or black. The septum cap was sealed using grease, and the mixture was stirred vigorously at –30 °C for 48 h. Then, the reaction was quenched by the addition of EtOH (1 mL), and the mixture was allowed to warm to r.t. Next, it was filtered through an Acrodisc®. The filtrate was concentrated under vacuum to a volume of approximately 1 mL, and the residue was purified by preparative TLC on silica to furnish the desired product.

A second run was performed with (*R*)-**1**.



(1-Cycloheptylpropyl)benzene (Table 2, entry 16). The title compound was prepared according to General Procedure 3, using (±)-(1-bromopropyl)benzene (199 mg, 1 mmol) and cycloheptylzinc iodide (0.7 M in 1,4-dioxane; 4.3 mL, 3.0 mmol). The reaction was stirred at –30 °C for 48 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the compound was isolated as a colorless oil.

1st run: 125 mg (58%, 85% ee); 2nd run: 132 mg (61% 88% ee).

The ee was determined by GC analysis (75→130 °C, ramp: 0.5 °C/min); retention times for compound obtained using (*S*)-**1**: t_r (major): 101.77 min, t_r (minor): 103.08 min.

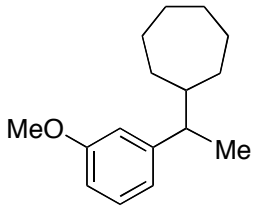
$[\alpha]^{25}_D = -9.4$ (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30-7.23 (m, 2 H), 7.20-7.14 (m, 1 H), 7.14-7.10 (m, 2 H), 2.35-2.28 (m, 1 H), 1.86-1.74 (m, 2 H), 1.74-1.48 (m, 7 H), 1.48-1.35 (m, 3 H), 1.35-1.15 (m, 2 H), 1.13-1.02 (m, 1 H), 0.71 (t, J = 7.4 Hz, 3 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.9, 128.9, 128.0, 125.7, 55.3, 44.4, 32.6, 32.0, 28.6, 28.3, 26.9, 26.8, 25.7, 12.7;

FT-IR (film): 3082, 3060, 3025, 2923, 2854, 1602, 1491, 1458, 1452, 1377, 1030, 901, 764 cm^{-1};

GC-MS (EI) calcd for $C_{16}H_{24}$ (M^+): 216, found: 216.



(1-Cycloheptylpropyl)-3-methoxybenzene (Table 2, entry 17). The title compound was prepared according to General Procedure 3, using (±)-(1-bromoethyl)-3-methoxybenzene (215 mg, 1 mmol) and cycloheptylzinc iodide (0.7 M in 1,4-dioxane; 4.3 mL, 3.0 mmol). The reaction was stirred at –30 °C for 48 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the compound was isolated as a colorless oil.

1st run: 119 mg (51%, 84% ee); 2nd run: 123 mg (53%, 83% ee).

The ee was determined by HPLC analysis, using an AD column; solvent system: 100% hexanes; flow rate: 1.0 mL/min; retention times for compound obtained using (*S*)-**1**: 10.34 min (minor), 11.39 min (major).

$[\alpha]^{25}_D$ = +3.3 (*c* = 1.0, $CHCl_3$; for compound obtained using (*S*)-**1**);

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.26-7.14 (m, 1 H), 6.82-6.66 (m, 3 H), 3.81 (s, 3 H), 2.57 (app pent, J = 7.1 Hz, 1 H), 1.84-1.73 (m, 1 H), 1.72-1.08 (m, 15 H);

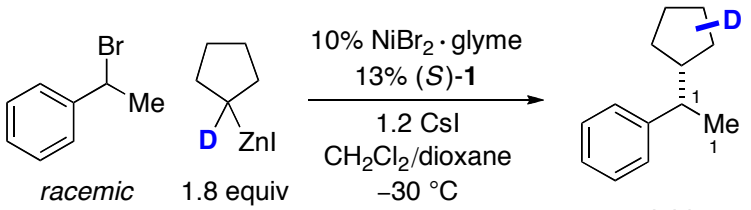
^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.4, 149.1, 128.8, 120.3, 113.8, 110.5, 55.1, 45.9, 45.4, 32.6, 31.2, 28.5, 28.2, 26.8, 26.6, 18.4;

FT-IR (film): 2921, 2853, 2833, 1609, 1600, 1582, 1486, 1456, 1435, 1375, 1282, 1260, 1153, 1045, 873, 854, 776 cm^{-1};

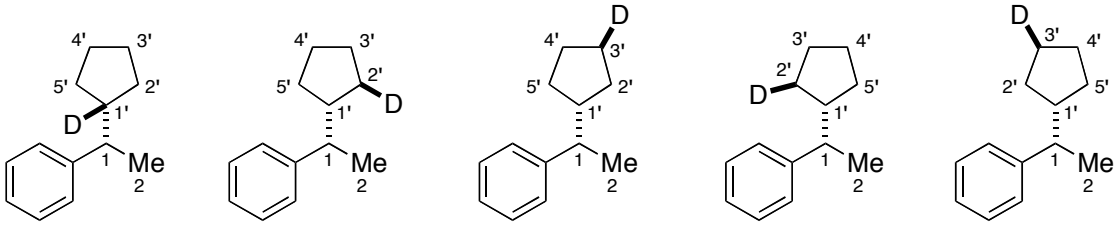
GC-MS (EI) calcd for $C_{16}H_{24}O$ (M^+): 232, found: 232.

Procedure for Equations 4 and 5. General Procedure 1 was employed, with isopropylzinc iodide or *n*-propylzinc iodide, instead of cyclopentylzinc iodide.

V. Mechanistic Study (eq 6)



93% yield
97% ee
five isomers:
D and 1-phenylethyl: *trans*



The reaction was performed on a 0.5 mmol scale according to General Procedure 1, using (±)-(1-bromoethyl)benzene (93 mg, 0.5 mmol) and 1-deuterocyclopentylzinc iodide (0.9 M in 1,4-dioxane; 1.0 mL, 0.9 mmol). The reaction was stirred at –30 °C for 48 h (both runs). After purification of the residue by preparative TLC on silica (100% hexanes), the products were isolated as an ~1:1:1:1:1 mixture of diastereo- (each is trans) and regioisomers as a colorless oil.

1st run: 85 mg (97%, 97% ee); 2nd run: 80 mg (92%, 98% ee).

The ee was determined by GC analysis using the method described for (1-cyclopentylethyl)benzene.

For clarity, integrals of ^{1}H NMR spectra have been quoted to the nearest integer.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.34-7.25 (m, 2 H), 7.22-7.15 (m, 3 H), 2.45 (dq, J = 9.6, 6.9 Hz, 1 H), 2.05-1.85 (m, 2 H), 1.75-1.37 (m, 5 H), 1.34-1.17 (m, 4 H), 1.10-0.97 (m, 1 H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.16, 128.26, 127.43, 125.80 (aromatic carbons are unresolved as distinct products), 47.75 (2C), 47.66 (2C), 47.20 (t, J = 19.3 Hz, A-C1′), 46.33 (4C), 46.22 (1C), 31.95 (2C), 31.85 (1C), 31.82 (1C), 31.60 (t, J = 20.9 Hz, B-C2′ or B′-C2′), 31.58 (2C), 31.48 (1C), 31.44 (1C), 31.23 (t, J = 20.5 Hz, B-C2′ or B′-C2′), 25.53 (1C), 25.51 (1C), 25.41 (1C), 25.39 (1C), 25.28 (1C), 25.26 (1C), 25.22 (t, J = 19.5 Hz, C-C3′ or C′-C3′), 25.17 (1C), 25.15 (1C), 24.90 (t, J = 19.5 Hz, C-C3′ or C′-C3′), 21.60 (4C), 21.56 (1C);

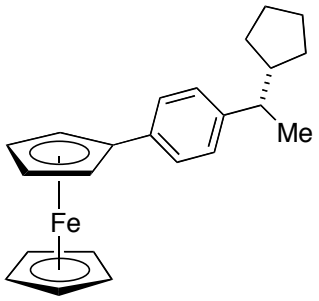
^{13}C{^{1}H, ^{2}H} NMR ($CDCl_3$, 125 MHz): δ 148.04, 128.15, 127.31, 125.68 (aromatic carbons are unresolved as distinct products), 47.64 (2C), 47.54 (2C), 47.08 (s, A-C1′), 46.2 (4C), 46.11 (1C), 31.84 (1C), 31.83 (1C), 31.74 (1C), 31.71 (1C), 31.48 (s, B-C2′ or B′-C2′), 31.47 (1C), 31.46 (1C), 31.37 (1C), 31.33 (1C), 31.11 (s, B-C2′ or B′-C2′), 25.42 (1C), 25.40 (1C), 25.30 (1C), 25.27 (1C), 25.16 (1C), 25.15 (1C), 25.05 (1C), 25.03 (2C; includes C-C3′ or C′-C3′), 24.78 (s, C-C3′ or C′-C3′), 21.49 (4C), 21.45 (1C);

^{2}H{^{1}H} NMR ($CHCl_3$, 60.6 MHz): δ 1.96 (s, 1 D), 1.91 (s, 1 D), 1.55 (s, 1 D), 1.44 (s, 1 D), 1.39 (s, 1 D);

FT-IR (film): 3082, 3061, 3025, 2953, 2870, 2165, 1602, 1492, 1451, 1373, 1302, 1078, 1014, 905, 761;

GC-MS (EI) calcd for $C_{13}H_{17}D$ (M^+): 175, found 175.

VI. Determination of Absolute Configuration



(*S*)-1-Ferrocenyl-4-(1-cyclopentylethyl)benzene. The title compound was prepared using a modification of a literature procedure.[4] In a glove box, a 20 mL oven-dried vial was charged with a stir bar, $Pd_2(dba)_3$ (27.5 mg, 0.030 mmol), ferroceneboronic acid (690 mg, 3.0 mmol), and potassium fluoride (384 mg, 6.6 mmol). A solution of P(*t*-Bu)$_3$ (18.2 mg, 0.090 mmol) in 1,4-dioxane (1 mL), prepared in a 4 mL vial, was added to the 20 mL vial, and the resulting mixture was stirred for 5 min. A solution of 1-chloro-4-(1-cyclopentylethyl)benzene (417 mg, 2.0 mmol), formed using the asymmetric cross-coupling method with ligand (*S*)-**1**, in THF (2 mL), prepared in a 4 mL vial, was transferred to the 20 mL vial; the 4 mL vial was rinsed with additional THF (1 mL), which was also transferred to the 20 mL vial. The 20 mL vial was capped, wrapped with electrical tape, removed from the glove box, and heated at 80 °C for 24 h. After cooling to r.t., the mixture was diluted with Et_2O (10 mL) and filtered through a short pad of silica, washing with additional Et_2O (~50 mL). The filtrate was concentrated under vacuum, absorbed onto silica, and purified by flash chromatography (100% hexanes), which furnished the product as a crystalline red solid (302 mg, 42%; not optimized). Recrystallization of the product from methanol yielded X-ray quality crystals, which established the absolute stereochemistry as *S*.

$[\alpha]^{25}_D$ = +24.9 (*c* = 1.0, $CHCl_3$);

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40 (d, *J* = 7.9 Hz, 2 H), 7.11 (d, *J* = 7.8 Hz, 2 H), 4.62 (s, 2 H), 4.29 (s, 2 H), 4.06 (s, 5 H), 2.43 (dt, *J* = 13.4, 6.9 Hz, 1 H), 1.95 (tdd, *J* = 18.2, 10.1, 4.6 Hz, 2 H), 1.74-1.56 (m, 3 H), 1.51-1.38 (m, 2 H), 1.32-1.18 (m, 4 H), 1.07 (tdd, *J* = 15.3, 10.6, 7.3 Hz, 1 H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 145.9, 136.4, 127.4, 126.1, 86.1, 69.6, 68.7, 66.5, 47.8, 45.9, 32.0, 31.6, 25.5, 25.3, 21.4.

FT-IR (film): 3094, 3057, 2953, 2867, 1611, 1527, 1456, 1420, 1410, 1372, 1279, 1104, 1082, 1022, 1001, 888, 835, 827, 813.

LC-MS (ES) calcd for $C_{23}H_{26}Fe$ (M^+): 358, found 358.

A crystal suitable for X-ray crystallography was grown by vapor diffusion with methanol.

(4) Littke, A. F.; Dai, C.; Fu, G. C. *J. Am. Chem. Soc.* **2000**, *122*, 4020–4028.

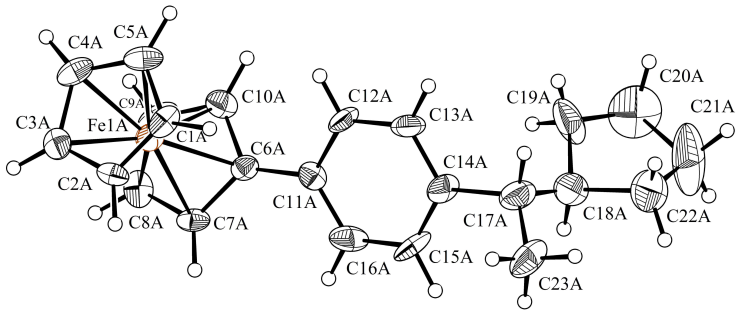


Table 1. Crystal Data and Structure Analysis Details for cjc01.

Empirical formula	C23 H26 Fe	
Formula weight	358.29	
Crystallization solvent	MeOH	
Crystal shape	block	
Crystal color	orange	
Crystal size	0.19 x 0.27 x 0.36 mm	
Data Collection:		
Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoK	
Data collection temperature	100 K	
Theta range for 9802 reflections used in lattice determination	2.21 to 29.23°	
Unit cell dimensions	a = 8.0625(3) Å	α = 90°
	b = 10.1789(4) Å	β = 92.733(2)°
	c = 43.7135(16) Å	γ = 90°
Volume	3583.4(2) $Å^3$	
Z	8	
Crystal system	Monoclinic	
Space group	P2(1) (# 4)	
Density (calculated)	1.328 g/cm^3	
F(000)	1520	
Theta range for data collection	1.4 to 29.5°	
Completeness to theta = 25.00°	99.9%	
Index ranges	$-11 \le h \le 10$, $-14 \le k \le 13$, $-58 \le l \le 59$	
Data collection scan type	narrow and scans	
Reflections collected	61669	
Independent reflections	18252 [R_{int}= 0.0386]	
Reflections > 2□(I)	14934	
Average □(I)/(net I)	0.0562	
Absorption coefficient	0.84 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8564 and 0.7515	
Reflections monitored for decay	0	

Decay of standards	0%

Structure Solution and Refinement:

Primary solution method	direct
Secondary solution method	difmap
Hydrogen placement	geom
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	18252 / 79 / 869
Treatment of hydrogen atoms	constr
Goodness-of-fit on F^2	2.12
Final R indices [I>2□(I), 14934 reflections]	R1 = 0.0668, wR2 = 0.0855
R indices (all data)	R1 = 0.0850, wR2 = 0.0873
Type of weighting scheme used	calc
Weighting scheme used	calc w=1/[^2^(Fo^2^)
Max shift/error	0.001
Average shift/error	0.000
Absolute structure parameter	0.032(17)
Largest diff. peak and hole	1.24 and -1.21 e·Å^{-3}

Programs Used:

Cell refinement	SAINT V8.18C (Bruker-AXS, 2007)
Data collection	Bruker SMART v5.054 (Bruker, 2007)
Data reduction	SAINT V8.18C (Bruker-AXS, 2007)
Structure solution	SHELXS-97 (Sheldrick, 1990)
Structure refinement	SHELXL-97 (Sheldrick, 1997)
Graphics	DIAMOND 3 (Crystal Impact, 1999)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for cjc01. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Fe(1A)	10669(1)	2280(1)	4483(1)	29(1)
C(1A)	11560(7)	3615(5)	4182(1)	29(1)
C(2A)	12772(7)	2637(6)	4256(1)	28(1)
C(3A)	13123(7)	2671(6)	4578(1)	32(1)
C(4A)	12126(8)	3688(6)	4701(1)	37(2)
C(5A)	11102(8)	4245(6)	4454(1)	35(2)
C(6A)	8607(7)	1463(6)	4271(1)	26(1)
C(7A)	9789(7)	468(6)	4352(1)	28(1)
C(8A)	10118(7)	507(6)	4674(1)	35(2)
C(9A)	9096(8)	1536(6)	4791(1)	39(2)
C(10A)	8203(8)	2117(6)	4546(1)	35(2)
C(11A)	7842(7)	1764(6)	3964(1)	27(2)
C(12A)	7263(7)	3009(6)	3892(1)	33(2)
C(13A)	6477(7)	3293(6)	3611(1)	40(2)
C(14A)	6275(8)	2343(6)	3391(1)	37(2)
C(15A)	6876(8)	1091(6)	3455(1)	38(2)
C(16A)	7632(8)	836(6)	3736(1)	40(2)
C(17A)	5275(9)	2596(7)	3089(1)	49(2)
C(18A)	3538(8)	2154(7)	3107(1)	48(2)
C(19A)	2579(8)	2785(8)	3359(1)	90(3)
C(20A)	888(9)	2660(9)	3281(1)	86(3)
C(21A)	725(9)	2383(9)	2924(2)	111(4)

C(22A)	2374(9)	2433(6)	2818(1)	73(2)
C(23A)	6095(6)	2093(4)	2807(1)	53(1)
Fe(1B)	-496(1)	9353(1)	577(1)	10(1)
C(1B)	-1308(6)	10708(5)	880(1)	16(1)
C(2B)	-2597(6)	9782(5)	806(1)	18(1)
C(3B)	-2960(6)	9826(5)	487(1)	16(1)
C(4B)	-1869(6)	10797(5)	360(1)	19(1)
C(5B)	-845(6)	11335(6)	603(1)	18(1)
C(6B)	1627(6)	8527(5)	779(1)	12(1)
C(7B)	365(5)	7542(5)	725(1)	9(1)
C(8B)	-64(6)	7519(5)	405(1)	15(1)
C(9B)	909(6)	8485(5)	257(1)	16(1)
C(10B)	1945(6)	9119(6)	491(1)	14(1)
C(11B)	2458(6)	8857(5)	1073(1)	12(1)
C(12B)	3033(6)	10136(5)	1135(1)	17(1)
C(13B)	3876(6)	10460(6)	1404(1)	20(1)
C(14B)	4188(7)	9528(6)	1632(1)	25(1)
C(15B)	3666(6)	8240(5)	1571(1)	17(1)
C(16B)	2814(6)	7917(5)	1297(1)	16(1)
C(17B)	5086(7)	9878(5)	1933(1)	26(1)
C(18B)	6845(5)	9319(4)	1965(1)	24(1)
C(19B)	7988(7)	9699(6)	1718(1)	40(2)
C(20B)	9769(7)	9505(6)	1845(1)	56(2)
C(21B)	9619(6)	9371(7)	2184(1)	80(2)
C(22B)	7852(5)	9736(5)	2254(1)	42(1)
C(23B)	4065(6)	9485(5)	2204(1)	45(1)
Fe(1C)	4403(1)	4688(1)	529(1)	10(1)
C(1C)	3659(6)	3354(5)	837(1)	21(1)
C(2C)	3923(6)	2731(5)	551(1)	17(1)
C(3C)	2906(6)	3290(5)	320(1)	14(1)
C(4C)	1924(6)	4255(6)	459(1)	14(1)
C(5C)	2365(6)	4272(6)	773(1)	17(1)
C(6C)	6500(6)	5542(5)	730(1)	12(1)
C(7C)	6852(6)	4898(5)	450(1)	10(1)
C(8C)	5863(6)	5472(5)	206(1)	11(1)
C(9C)	4897(6)	6473(5)	332(1)	11(1)
C(10C)	5268(6)	6525(5)	649(1)	14(1)
C(11C)	7234(6)	5269(5)	1037(1)	12(1)
C(12C)	7328(6)	6259(5)	1261(1)	12(1)
C(13C)	8172(7)	6033(5)	1540(1)	24(1)
C(14C)	8941(6)	4829(5)	1615(1)	20(1)
C(15C)	8794(7)	3855(6)	1388(1)	28(1)
C(16C)	7975(6)	4055(5)	1108(1)	23(1)
C(17C)	9954(7)	4653(6)	1911(1)	32(2)
C(18C)	11815(7)	4915(6)	1858(1)	30(1)
C(19C)	12875(6)	5186(5)	2145(1)	37(1)
C(20C)	14683(6)	4815(5)	2064(1)	31(1)
C(21C)	14512(7)	4100(6)	1764(1)	47(2)
C(22C)	12722(6)	3766(6)	1710(1)	48(2)
C(23C)	9523(6)	3419(5)	2078(1)	61(2)
Fe(1D)	5457(1)	7609(1)	4409(1)	29(1)
C(1D)	6166(7)	6181(6)	4120(2)	36(2)
C(2D)	5818(8)	5636(6)	4405(2)	43(2)
C(3D)	6862(8)	6192(6)	4628(1)	40(2)
C(4D)	7870(7)	7102(6)	4484(2)	39(2)
C(5D)	7462(7)	7093(6)	4172(1)	30(2)

C(6D)	3387(7)	8483(6)	4208(1)	26(1)
C(7D)	3057(7)	7936(6)	4499(1)	30(2)
C(8D)	4097(7)	8525(6)	4724(1)	31(2)
C(9D)	5107(7)	9453(6)	4581(1)	33(2)
C(10D)	4662(7)	9435(6)	4266(1)	36(2)
C(11D)	2514(7)	8155(6)	3909(1)	28(2)
C(12D)	2296(7)	9077(6)	3677(1)	39(2)
C(13D)	1427(8)	8771(7)	3405(1)	45(2)
C(14D)	746(7)	7535(7)	3352(1)	32(2)
C(15D)	983(7)	6639(7)	3577(1)	45(2)
C(16D)	1845(7)	6905(6)	3859(2)	40(2)
C(17D)	-170(7)	7196(7)	3045(1)	45(2)
C(18D)	-1792(5)	6597(5)	3077(1)	37(1)
C(19D)	-3008(8)	7292(7)	3275(2)	57(2)
C(20D)	-4592(9)	7251(11)	3110(2)	182(6)
C(21D)	-4538(6)	6589(5)	2820(1)	50(2)
C(22D)	-2759(6)	6347(5)	2766(1)	50(2)
C(23D)	994(7)	6485(9)	2839(1)	130(4)

Table 3. Bond lengths [Å] and angles [°] for cjc01.

Fe(1A)-C(10A)	2.027(6)
Fe(1A)-C(5A)	2.035(6)
Fe(1A)-C(9A)	2.037(6)
Fe(1A)-C(2A)	2.039(6)
Fe(1A)-C(3A)	2.041(6)
Fe(1A)-C(6A)	2.042(6)
Fe(1A)-C(1A)	2.046(5)
Fe(1A)-C(8A)	2.047(6)
Fe(1A)-C(7A)	2.049(6)
Fe(1A)-C(4A)	2.056(6)
C(1A)-C(5A)	1.415(7)
C(1A)-C(2A)	1.421(8)
C(1A)-H(1A)	1.0000
C(2A)-C(3A)	1.424(7)
C(2A)-H(2A)	1.0000
C(3A)-C(4A)	1.430(8)
C(3A)-H(3A)	1.0000
C(4A)-C(5A)	1.443(8)
C(4A)-H(4A)	1.0000
C(5A)-H(5A)	1.0000
C(6A)-C(7A)	1.423(8)
C(6A)-C(10A)	1.425(8)
C(6A)-C(11A)	1.484(8)
C(7A)-C(8A)	1.423(8)
C(7A)-H(7A)	1.0000
C(8A)-C(9A)	1.441(8)
C(8A)-H(8A)	1.0000
C(9A)-C(10A)	1.392(8)
C(9A)-H(9A)	1.0000
C(10A)-H(10A)	1.0000
C(11A)-C(16A)	1.379(8)
C(11A)-C(12A)	1.381(8)
C(12A)-C(13A)	1.387(7)
C(12A)-H(12A)	0.9500
C(13A)-C(14A)	1.367(7)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.387(8)
C(14A)-C(17A)	1.535(8)
C(15A)-C(16A)	1.369(8)
C(15A)-H(15A)	0.9500
C(16A)-H(16A)	0.9500
C(17A)-C(18A)	1.477(8)
C(17A)-C(23A)	1.514(7)
C(17A)-H(17A)	1.0000
C(18A)-C(19A)	1.517(8)
C(18A)-C(22A)	1.563(8)
C(18A)-H(18A)	1.0000
C(19A)-C(20A)	1.395(8)
C(19A)-H(19A)	0.9900
C(19A)-H(19B)	0.9900
C(20A)-C(21A)	1.584(8)
C(20A)-H(20A)	0.9900
C(20A)-H(20B)	0.9900
C(21A)-C(22A)	1.429(8)

C(21A)-H(21A)	0.9900
C(21A)-H(21B)	0.9900
C(22A)-H(22A)	0.9900
C(22A)-H(22B)	0.9900
C(23A)-H(23A)	0.9800
C(23A)-H(23B)	0.9800
C(23A)-H(23C)	0.9800
Fe(1B)-C(10B)	2.035(5)
Fe(1B)-C(5B)	2.041(6)
Fe(1B)-C(1B)	2.042(5)
Fe(1B)-C(9B)	2.043(5)
Fe(1B)-C(4B)	2.047(5)
Fe(1B)-C(8B)	2.048(5)
Fe(1B)-C(2B)	2.056(5)
Fe(1B)-C(7B)	2.063(5)
Fe(1B)-C(3B)	2.064(5)
Fe(1B)-C(6B)	2.066(5)
C(1B)-C(2B)	1.429(7)
C(1B)-C(5B)	1.435(6)
C(1B)-H(1B)	1.0000
C(2B)-C(3B)	1.413(7)
C(2B)-H(2B)	1.0000
C(3B)-C(4B)	1.451(7)
C(3B)-H(3B)	1.0000
C(4B)-C(5B)	1.424(7)
C(4B)-H(4B)	1.0000
C(5B)-H(5B)	1.0000
C(6B)-C(10B)	1.428(6)
C(6B)-C(7B)	1.440(6)
C(6B)-C(11B)	1.463(7)
C(7B)-C(8B)	1.425(6)
C(7B)-H(7B)	1.0000
C(8B)-C(9B)	1.432(6)
C(8B)-H(8B)	1.0000
C(9B)-C(10B)	1.442(6)
C(9B)-H(9B)	1.0000
C(10B)-H(10B)	1.0000
C(11B)-C(16B)	1.389(6)
C(11B)-C(12B)	1.404(7)
C(12B)-C(13B)	1.372(7)
C(12B)-H(12B)	0.9500
C(13B)-C(14B)	1.388(7)
C(13B)-H(13B)	0.9500
C(14B)-C(15B)	1.398(7)
C(14B)-C(17B)	1.514(7)
C(15B)-C(16B)	1.392(6)
C(15B)-H(15B)	0.9500
C(16B)-H(16B)	0.9500
C(17B)-C(18B)	1.528(6)
C(17B)-C(23B)	1.529(7)
C(17B)-H(17B)	1.0000
C(18B)-C(19B)	1.503(6)
C(18B)-C(22B)	1.530(5)
C(18B)-H(18B)	1.0000
C(19B)-C(20B)	1.527(8)
C(19B)-H(19C)	0.9900

C(19B)-H(19D)	0.9900
C(20B)-C(21B)	1.497(7)
C(20B)-H(20C)	0.9900
C(20B)-H(20D)	0.9900
C(21B)-C(22B)	1.518(6)
C(21B)-H(21C)	0.9900
C(21B)-H(21D)	0.9900
C(22B)-H(22C)	0.9900
C(22B)-H(22D)	0.9900
C(23B)-H(23D)	0.9800
C(23B)-H(23E)	0.9800
C(23B)-H(23F)	0.9800
Fe(1C)-C(1C)	2.021(5)
Fe(1C)-C(2C)	2.031(5)
Fe(1C)-C(7C)	2.032(5)
Fe(1C)-C(5C)	2.044(5)
Fe(1C)-C(8C)	2.046(5)
Fe(1C)-C(3C)	2.053(5)
Fe(1C)-C(10C)	2.055(5)
Fe(1C)-C(4C)	2.056(5)
Fe(1C)-C(6C)	2.059(5)
Fe(1C)-C(9C)	2.059(5)
C(1C)-C(5C)	1.418(7)
C(1C)-C(2C)	1.426(6)
C(1C)-H(1C)	1.0000
C(2C)-C(3C)	1.393(6)
C(2C)-H(2C)	1.0000
C(3C)-C(4C)	1.416(6)
C(3C)-H(3C)	1.0000
C(4C)-C(5C)	1.402(6)
C(4C)-H(4C)	1.0000
C(5C)-H(5C)	1.0000
C(6C)-C(7C)	1.427(7)
C(6C)-C(10C)	1.442(7)
C(6C)-C(11C)	1.467(7)
C(7C)-C(8C)	1.429(6)
C(7C)-H(7C)	1.0000
C(8C)-C(9C)	1.410(6)
C(8C)-H(8C)	1.0000
C(9C)-C(10C)	1.407(6)
C(9C)-H(9C)	1.0000
C(10C)-H(10C)	1.0000
C(11C)-C(16C)	1.401(7)
C(11C)-C(12C)	1.405(6)
C(12C)-C(13C)	1.387(6)
C(12C)-H(12C)	0.9500
C(13C)-C(14C)	1.405(7)
C(13C)-H(13C)	0.9500
C(14C)-C(15C)	1.405(7)
C(14C)-C(17C)	1.509(7)
C(15C)-C(16C)	1.375(7)
C(15C)-H(15C)	0.9500
C(16C)-H(16C)	0.9500
C(17C)-C(23C)	1.500(7)
C(17C)-C(18C)	1.552(7)
C(17C)-H(17C)	1.0000

C(18C)-C(19C)	1.508(7)
C(18C)-C(22C)	1.539(7)
C(18C)-H(18C)	1.0000
C(19C)-C(20C)	1.562(6)
C(19C)-H(19E)	0.9900
C(19C)-H(19F)	0.9900
C(20C)-C(21C)	1.501(7)
C(20C)-H(20E)	0.9900
C(20C)-H(20F)	0.9900
C(21C)-C(22C)	1.491(7)
C(21C)-H(21E)	0.9900
C(21C)-H(21F)	0.9900
C(22C)-H(22E)	0.9900
C(22C)-H(22F)	0.9900
C(23C)-H(23G)	0.9800
C(23C)-H(23H)	0.9800
C(23C)-H(23I)	0.9800
Fe(1D)-C(7D)	2.021(6)
Fe(1D)-C(1D)	2.024(6)
Fe(1D)-C(4D)	2.025(6)
Fe(1D)-C(2D)	2.029(6)
Fe(1D)-C(5D)	2.030(6)
Fe(1D)-C(8D)	2.030(6)
Fe(1D)-C(3D)	2.045(6)
Fe(1D)-C(9D)	2.048(6)
Fe(1D)-C(6D)	2.051(5)
Fe(1D)-C(10D)	2.054(6)
C(1D)-C(2D)	1.402(8)
C(1D)-C(5D)	1.408(8)
C(1D)-H(1D)	1.0000
C(2D)-C(3D)	1.381(8)
C(2D)-H(2D)	1.0000
C(3D)-C(4D)	1.401(8)
C(3D)-H(3D)	1.0000
C(4D)-C(5D)	1.390(8)
C(4D)-H(4D)	1.0000
C(5D)-H(5D)	1.0000
C(6D)-C(7D)	1.422(7)
C(6D)-C(10D)	1.427(8)
C(6D)-C(11D)	1.492(7)
C(7D)-C(8D)	1.399(7)
C(7D)-H(7D)	1.0000
C(8D)-C(9D)	1.412(8)
C(8D)-H(8D)	1.0000
C(9D)-C(10D)	1.408(8)
C(9D)-H(9D)	1.0000
C(10D)-H(10D)	1.0000
C(11D)-C(12D)	1.388(7)
C(11D)-C(16D)	1.396(8)
C(12D)-C(13D)	1.386(8)
C(12D)-H(12D)	0.9500
C(13D)-C(14D)	1.389(9)
C(13D)-H(13D)	0.9500
C(14D)-C(15D)	1.350(8)
C(14D)-C(17D)	1.537(7)
C(15D)-C(16D)	1.410(8)

C(15D)-H(15D)	0.9500
C(16D)-H(16D)	0.9500
C(17D)-C(18D)	1.456(7)
C(17D)-C(23D)	1.516(8)
C(17D)-H(17D)	1.0000
C(18D)-C(19D)	1.512(7)
C(18D)-C(22D)	1.555(5)
C(18D)-H(18D)	1.0000
C(19D)-C(20D)	1.437(9)
C(19D)-H(19G)	0.9900
C(19D)-H(19H)	0.9900
C(20D)-C(21D)	1.438(7)
C(20D)-H(20G)	0.9900
C(20D)-H(20H)	0.9900
C(21D)-C(22D)	1.485(6)
C(21D)-H(21G)	0.9900
C(21D)-H(21H)	0.9900
C(22D)-H(22G)	0.9900
C(22D)-H(22H)	0.9900
C(23D)-H(23J)	0.9800
C(23D)-H(23K)	0.9800
C(23D)-H(23L)	0.9800

C(10A)-Fe(1A)-C(5A)	105.2(3)
C(10A)-Fe(1A)-C(9A)	40.0(2)
C(5A)-Fe(1A)-C(9A)	121.4(2)
C(10A)-Fe(1A)-C(2A)	157.7(2)
C(5A)-Fe(1A)-C(2A)	69.2(2)
C(9A)-Fe(1A)-C(2A)	161.1(3)
C(10A)-Fe(1A)-C(3A)	159.4(2)
C(5A)-Fe(1A)-C(3A)	69.8(3)
C(9A)-Fe(1A)-C(3A)	124.5(3)
C(2A)-Fe(1A)-C(3A)	40.9(2)
C(10A)-Fe(1A)-C(6A)	41.0(2)
C(5A)-Fe(1A)-C(6A)	120.7(3)
C(9A)-Fe(1A)-C(6A)	68.2(2)
C(2A)-Fe(1A)-C(6A)	122.0(2)
C(3A)-Fe(1A)-C(6A)	158.8(2)
C(10A)-Fe(1A)-C(1A)	121.3(2)
C(5A)-Fe(1A)-C(1A)	40.6(2)
C(9A)-Fe(1A)-C(1A)	157.0(3)
C(2A)-Fe(1A)-C(1A)	40.7(2)
C(3A)-Fe(1A)-C(1A)	68.6(2)
C(6A)-Fe(1A)-C(1A)	106.3(2)
C(10A)-Fe(1A)-C(8A)	68.8(2)
C(5A)-Fe(1A)-C(8A)	159.0(2)
C(9A)-Fe(1A)-C(8A)	41.3(2)
C(2A)-Fe(1A)-C(8A)	123.9(3)
C(3A)-Fe(1A)-C(8A)	108.4(2)
C(6A)-Fe(1A)-C(8A)	68.8(2)
C(1A)-Fe(1A)-C(8A)	159.7(2)
C(10A)-Fe(1A)-C(7A)	68.6(2)
C(5A)-Fe(1A)-C(7A)	157.7(2)
C(9A)-Fe(1A)-C(7A)	68.4(2)
C(2A)-Fe(1A)-C(7A)	108.0(2)
C(3A)-Fe(1A)-C(7A)	123.5(2)

C(6A)-Fe(1A)-C(7A)	40.7(2)
C(1A)-Fe(1A)-C(7A)	123.0(2)
C(8A)-Fe(1A)-C(7A)	40.7(2)
C(10A)-Fe(1A)-C(4A)	122.5(3)
C(5A)-Fe(1A)-C(4A)	41.3(2)
C(9A)-Fe(1A)-C(4A)	108.3(2)
C(2A)-Fe(1A)-C(4A)	68.3(2)
C(3A)-Fe(1A)-C(4A)	40.8(2)
C(6A)-Fe(1A)-C(4A)	158.2(3)
C(1A)-Fe(1A)-C(4A)	67.9(2)
C(8A)-Fe(1A)-C(4A)	123.8(2)
C(7A)-Fe(1A)-C(4A)	159.9(3)
C(5A)-C(1A)-C(2A)	109.3(5)
C(5A)-C(1A)-Fe(1A)	69.3(3)
C(2A)-C(1A)-Fe(1A)	69.3(3)
C(5A)-C(1A)-H(1A)	125.3
C(2A)-C(1A)-H(1A)	125.3
Fe(1A)-C(1A)-H(1A)	125.3
C(1A)-C(2A)-C(3A)	108.1(5)
C(1A)-C(2A)-Fe(1A)	69.9(3)
C(3A)-C(2A)-Fe(1A)	69.7(3)
C(1A)-C(2A)-H(2A)	126.0
C(3A)-C(2A)-H(2A)	126.0
Fe(1A)-C(2A)-H(2A)	126.0
C(2A)-C(3A)-C(4A)	107.4(6)
C(2A)-C(3A)-Fe(1A)	69.5(3)
C(4A)-C(3A)-Fe(1A)	70.1(3)
C(2A)-C(3A)-H(3A)	126.3
C(4A)-C(3A)-H(3A)	126.3
Fe(1A)-C(3A)-H(3A)	126.3
C(3A)-C(4A)-C(5A)	108.5(5)
C(3A)-C(4A)-Fe(1A)	69.0(3)
C(5A)-C(4A)-Fe(1A)	68.6(3)
C(3A)-C(4A)-H(4A)	125.7
C(5A)-C(4A)-H(4A)	125.7
Fe(1A)-C(4A)-H(4A)	125.7
C(1A)-C(5A)-C(4A)	106.7(6)
C(1A)-C(5A)-Fe(1A)	70.1(3)
C(4A)-C(5A)-Fe(1A)	70.1(3)
C(1A)-C(5A)-H(5A)	126.6
C(4A)-C(5A)-H(5A)	126.6
Fe(1A)-C(5A)-H(5A)	126.6
C(7A)-C(6A)-C(10A)	107.5(5)
C(7A)-C(6A)-C(11A)	128.0(6)
C(10A)-C(6A)-C(11A)	124.4(6)
C(7A)-C(6A)-Fe(1A)	69.9(3)
C(10A)-C(6A)-Fe(1A)	68.9(3)
C(11A)-C(6A)-Fe(1A)	128.4(4)
C(8A)-C(7A)-C(6A)	108.5(5)
C(8A)-C(7A)-Fe(1A)	69.6(3)
C(6A)-C(7A)-Fe(1A)	69.4(3)
C(8A)-C(7A)-H(7A)	125.8
C(6A)-C(7A)-H(7A)	125.8
Fe(1A)-C(7A)-H(7A)	125.8
C(7A)-C(8A)-C(9A)	106.7(5)
C(7A)-C(8A)-Fe(1A)	69.7(3)

C(9A)-C(8A)-Fe(1A) 69.0(3)
C(7A)-C(8A)-H(8A) 126.6
C(9A)-C(8A)-H(8A) 126.6
Fe(1A)-C(8A)-H(8A) 126.6
C(10A)-C(9A)-C(8A) 108.7(5)
C(10A)-C(9A)-Fe(1A) 69.6(4)
C(8A)-C(9A)-Fe(1A) 69.7(3)
C(10A)-C(9A)-H(9A) 125.6
C(8A)-C(9A)-H(9A) 125.6
Fe(1A)-C(9A)-H(9A) 125.6
C(9A)-C(10A)-C(6A) 108.6(6)
C(9A)-C(10A)-Fe(1A) 70.4(4)
C(6A)-C(10A)-Fe(1A) 70.0(3)
C(9A)-C(10A)-H(10A) 125.7
C(6A)-C(10A)-H(10A) 125.7
Fe(1A)-C(10A)-H(10A)125.7
C(16A)-C(11A)-C(12A)115.9(5)
C(16A)-C(11A)-C(6A) 123.0(6)
C(12A)-C(11A)-C(6A) 121.1(6)
C(11A)-C(12A)-C(13A)121.8(6)
C(11A)-C(12A)-H(12A)119.1
C(13A)-C(12A)-H(12A)119.1
C(14A)-C(13A)-C(12A)120.7(6)
C(14A)-C(13A)-H(13A)119.7
C(12A)-C(13A)-H(13A)119.7
C(13A)-C(14A)-C(15A)118.7(6)
C(13A)-C(14A)-C(17A)121.7(6)
C(15A)-C(14A)-C(17A)119.4(6)
C(16A)-C(15A)-C(14A)119.4(6)
C(16A)-C(15A)-H(15A)120.3
C(14A)-C(15A)-H(15A)120.3
C(15A)-C(16A)-C(11A)123.5(6)
C(15A)-C(16A)-H(16A)118.2
C(11A)-C(16A)-H(16A)118.2
C(18A)-C(17A)-C(23A)113.1(5)
C(18A)-C(17A)-C(14A)111.3(6)
C(23A)-C(17A)-C(14A)114.2(5)
C(18A)-C(17A)-H(17A)105.8
C(23A)-C(17A)-H(17A)105.8
C(14A)-C(17A)-H(17A)105.8
C(17A)-C(18A)-C(19A)115.3(6)
C(17A)-C(18A)-C(22A)115.8(6)
C(19A)-C(18A)-C(22A)101.6(5)
C(17A)-C(18A)-H(18A)107.9
C(19A)-C(18A)-H(18A)107.9
C(22A)-C(18A)-H(18A)107.9
C(20A)-C(19A)-C(18A)108.0(6)
C(20A)-C(19A)-H(19A)110.1
C(18A)-C(19A)-H(19A)110.1
C(20A)-C(19A)-H(19B)110.1
C(18A)-C(19A)-H(19B)110.1
H(19A)-C(19A)-H(19B)108.4
C(19A)-C(20A)-C(21A)106.9(5)
C(19A)-C(20A)-H(20A)110.3
C(21A)-C(20A)-H(20A)110.3
C(19A)-C(20A)-H(20B)110.3

C(21A)-C(20A)-H(20B)110.3
H(20A)-C(20A)-H(20B)108.6
C(22A)-C(21A)-C(20A)106.1(6)
C(22A)-C(21A)-H(21A)110.5
C(20A)-C(21A)-H(21A)110.5
C(22A)-C(21A)-H(21B)110.5
C(20A)-C(21A)-H(21B)110.5
H(21A)-C(21A)-H(21B)108.7
C(21A)-C(22A)-C(18A)105.3(5)
C(21A)-C(22A)-H(22A)110.7
C(18A)-C(22A)-H(22A)110.7
C(21A)-C(22A)-H(22B)110.7
C(18A)-C(22A)-H(22B)110.7
H(22A)-C(22A)-H(22B)108.8
C(17A)-C(23A)-H(23A)109.5
C(17A)-C(23A)-H(23B)109.5
H(23A)-C(23A)-H(23B)109.5
C(17A)-C(23A)-H(23C)109.5
H(23A)-C(23A)-H(23C)109.5
H(23B)-C(23A)-H(23C)109.5
C(10B)-Fe(1B)-C(5B) 105.3(2)
C(10B)-Fe(1B)-C(1B) 122.8(2)
C(5B)-Fe(1B)-C(1B) 41.15(18)
C(10B)-Fe(1B)-C(9B) 41.42(18)
C(5B)-Fe(1B)-C(9B) 123.2(2)
C(1B)-Fe(1B)-C(9B) 160.4(2)
C(10B)-Fe(1B)-C(4B) 120.3(2)
C(5B)-Fe(1B)-C(4B) 40.77(18)
C(1B)-Fe(1B)-C(4B) 68.5(2)
C(9B)-Fe(1B)-C(4B) 107.4(2)
C(10B)-Fe(1B)-C(8B) 69.1(2)
C(5B)-Fe(1B)-C(8B) 161.4(2)
C(1B)-Fe(1B)-C(8B) 156.8(2)
C(9B)-Fe(1B)-C(8B) 40.98(18)
C(4B)-Fe(1B)-C(8B) 125.6(2)
C(10B)-Fe(1B)-C(2B) 160.3(2)
C(5B)-Fe(1B)-C(2B) 69.1(2)
C(1B)-Fe(1B)-C(2B) 40.80(19)
C(9B)-Fe(1B)-C(2B) 157.3(2)
C(4B)-Fe(1B)-C(2B) 68.5(2)
C(8B)-Fe(1B)-C(2B) 122.0(2)
C(10B)-Fe(1B)-C(7B) 68.9(2)
C(5B)-Fe(1B)-C(7B) 155.67(19)
C(1B)-Fe(1B)-C(7B) 120.90(19)
C(9B)-Fe(1B)-C(7B) 68.85(19)
C(4B)-Fe(1B)-C(7B) 162.52(19)
C(8B)-Fe(1B)-C(7B) 40.55(17)
C(2B)-Fe(1B)-C(7B) 108.04(19)
C(10B)-Fe(1B)-C(3B) 157.29(19)
C(5B)-Fe(1B)-C(3B) 69.3(2)
C(1B)-Fe(1B)-C(3B) 68.3(2)
C(9B)-Fe(1B)-C(3B) 122.0(2)
C(4B)-Fe(1B)-C(3B) 41.36(18)
C(8B)-Fe(1B)-C(3B) 108.7(2)
C(2B)-Fe(1B)-C(3B) 40.12(19)
C(7B)-Fe(1B)-C(3B) 125.1(2)

C(10B)-Fe(1B)-C(6B)	40.77(18)
C(5B)-Fe(1B)-C(6B)	119.5(2)
C(1B)-Fe(1B)-C(6B)	106.4(2)
C(9B)-Fe(1B)-C(6B)	68.96(19)
C(4B)-Fe(1B)-C(6B)	155.4(2)
C(8B)-Fe(1B)-C(6B)	68.51(19)
C(2B)-Fe(1B)-C(6B)	124.3(2)
C(7B)-Fe(1B)-C(6B)	40.81(17)
C(3B)-Fe(1B)-C(6B)	161.2(2)
C(2B)-C(1B)-C(5B)	108.5(5)
C(2B)-C(1B)-Fe(1B)	70.1(3)
C(5B)-C(1B)-Fe(1B)	69.4(3)
C(2B)-C(1B)-H(1B)	125.7
C(5B)-C(1B)-H(1B)	125.7
Fe(1B)-C(1B)-H(1B)	125.7
C(3B)-C(2B)-C(1B)	108.5(5)
C(3B)-C(2B)-Fe(1B)	70.2(3)
C(1B)-C(2B)-Fe(1B)	69.1(3)
C(3B)-C(2B)-H(2B)	125.8
C(1B)-C(2B)-H(2B)	125.8
Fe(1B)-C(2B)-H(2B)	125.8
C(2B)-C(3B)-C(4B)	107.4(5)
C(2B)-C(3B)-Fe(1B)	69.7(3)
C(4B)-C(3B)-Fe(1B)	68.7(3)
C(2B)-C(3B)-H(3B)	126.3
C(4B)-C(3B)-H(3B)	126.3
Fe(1B)-C(3B)-H(3B)	126.3
C(5B)-C(4B)-C(3B)	108.5(5)
C(5B)-C(4B)-Fe(1B)	69.4(3)
C(3B)-C(4B)-Fe(1B)	70.0(3)
C(5B)-C(4B)-H(4B)	125.8
C(3B)-C(4B)-H(4B)	125.8
Fe(1B)-C(4B)-H(4B)	125.8
C(4B)-C(5B)-C(1B)	107.1(5)
C(4B)-C(5B)-Fe(1B)	69.8(3)
C(1B)-C(5B)-Fe(1B)	69.5(3)
C(4B)-C(5B)-H(5B)	126.4
C(1B)-C(5B)-H(5B)	126.4
Fe(1B)-C(5B)-H(5B)	126.4
C(10B)-C(6B)-C(7B)	107.8(4)
C(10B)-C(6B)-C(11B)	125.7(5)
C(7B)-C(6B)-C(11B)	126.4(5)
C(10B)-C(6B)-Fe(1B)	68.5(3)
C(7B)-C(6B)-Fe(1B)	69.5(3)
C(11B)-C(6B)-Fe(1B)	128.1(4)
C(8B)-C(7B)-C(6B)	107.9(4)
C(8B)-C(7B)-Fe(1B)	69.2(3)
C(6B)-C(7B)-Fe(1B)	69.7(3)
C(8B)-C(7B)-H(7B)	126.0
C(6B)-C(7B)-H(7B)	126.0
Fe(1B)-C(7B)-H(7B)	126.0
C(7B)-C(8B)-C(9B)	108.7(5)
C(7B)-C(8B)-Fe(1B)	70.3(3)
C(9B)-C(8B)-Fe(1B)	69.3(3)
C(7B)-C(8B)-H(8B)	125.7
C(9B)-C(8B)-H(8B)	125.7

Fe(1B)-C(8B)-H(8B)	125.7
C(8B)-C(9B)-C(10B)	107.3(5)
C(8B)-C(9B)-Fe(1B)	69.7(3)
C(10B)-C(9B)-Fe(1B)	69.0(3)
C(8B)-C(9B)-H(9B)	126.3
C(10B)-C(9B)-H(9B)	126.3
Fe(1B)-C(9B)-H(9B)	126.3
C(6B)-C(10B)-C(9B)	108.2(5)
C(6B)-C(10B)-Fe(1B)	70.8(3)
C(9B)-C(10B)-Fe(1B)	69.6(3)
C(6B)-C(10B)-H(10B)	125.9
C(9B)-C(10B)-H(10B)	125.9
Fe(1B)-C(10B)-H(10B)	125.9
C(16B)-C(11B)-C(12B)	116.7(5)
C(16B)-C(11B)-C(6B)	122.2(5)
C(12B)-C(11B)-C(6B)	121.0(5)
C(13B)-C(12B)-C(11B)	122.2(5)
C(13B)-C(12B)-H(12B)	118.9
C(11B)-C(12B)-H(12B)	118.9
C(12B)-C(13B)-C(14B)	121.1(5)
C(12B)-C(13B)-H(13B)	119.5
C(14B)-C(13B)-H(13B)	119.5
C(13B)-C(14B)-C(15B)	117.6(5)
C(13B)-C(14B)-C(17B)	121.6(5)
C(15B)-C(14B)-C(17B)	120.8(5)
C(16B)-C(15B)-C(14B)	121.0(5)
C(16B)-C(15B)-H(15B)	119.5
C(14B)-C(15B)-H(15B)	119.5
C(11B)-C(16B)-C(15B)	121.4(5)
C(11B)-C(16B)-H(16B)	119.3
C(15B)-C(16B)-H(16B)	119.3
C(14B)-C(17B)-C(18B)	113.3(4)
C(14B)-C(17B)-C(23B)	111.1(4)
C(18B)-C(17B)-C(23B)	111.3(4)
C(14B)-C(17B)-H(17B)	106.9
C(18B)-C(17B)-H(17B)	106.9
C(23B)-C(17B)-H(17B)	106.9
C(19B)-C(18B)-C(17B)	115.9(4)
C(19B)-C(18B)-C(22B)	101.7(4)
C(17B)-C(18B)-C(22B)	115.2(4)
C(19B)-C(18B)-H(18B)	107.9
C(17B)-C(18B)-H(18B)	107.9
C(22B)-C(18B)-H(18B)	107.9
C(18B)-C(19B)-C(20B)	107.7(5)
C(18B)-C(19B)-H(19C)	110.2
C(20B)-C(19B)-H(19C)	110.2
C(18B)-C(19B)-H(19D)	110.2
C(20B)-C(19B)-H(19D)	110.2
H(19C)-C(19B)-H(19D)	108.5
C(21B)-C(20B)-C(19B)	104.6(4)
C(21B)-C(20B)-H(20C)	110.8
C(19B)-C(20B)-H(20C)	110.8
C(21B)-C(20B)-H(20D)	110.8
C(19B)-C(20B)-H(20D)	110.8
H(20C)-C(20B)-H(20D)	108.9
C(20B)-C(21B)-C(22B)	107.4(4)

C(20B)-C(21B)-H(21C)	110.2
C(22B)-C(21B)-H(21C)	110.2
C(20B)-C(21B)-H(21D)	110.2
C(22B)-C(21B)-H(21D)	110.2
H(21C)-C(21B)-H(21D)	108.5
C(21B)-C(22B)-C(18B)	103.3(4)
C(21B)-C(22B)-H(22C)	111.1
C(18B)-C(22B)-H(22C)	111.1
C(21B)-C(22B)-H(22D)	111.1
C(18B)-C(22B)-H(22D)	111.1
H(22C)-C(22B)-H(22D)	109.1
C(17B)-C(23B)-H(23D)	109.5
C(17B)-C(23B)-H(23E)	109.5
H(23D)-C(23B)-H(23E)	109.5
C(17B)-C(23B)-H(23F)	109.5
H(23D)-C(23B)-H(23F)	109.5
H(23E)-C(23B)-H(23F)	109.5
C(1C)-Fe(1C)-C(2C)	41.19(18)
C(1C)-Fe(1C)-C(7C)	120.4(2)
C(2C)-Fe(1C)-C(7C)	107.4(2)
C(1C)-Fe(1C)-C(5C)	40.8(2)
C(2C)-Fe(1C)-C(5C)	67.3(2)
C(7C)-Fe(1C)-C(5C)	157.2(2)
C(1C)-Fe(1C)-C(8C)	157.1(2)
C(2C)-Fe(1C)-C(8C)	122.1(2)
C(7C)-Fe(1C)-C(8C)	41.04(17)
C(5C)-Fe(1C)-C(8C)	160.8(2)
C(1C)-Fe(1C)-C(3C)	69.2(2)
C(2C)-Fe(1C)-C(3C)	39.87(18)
C(7C)-Fe(1C)-C(3C)	123.6(2)
C(5C)-Fe(1C)-C(3C)	67.6(2)
C(8C)-Fe(1C)-C(3C)	107.88(19)
C(1C)-Fe(1C)-C(10C)	123.4(2)
C(2C)-Fe(1C)-C(10C)	160.59(19)
C(7C)-Fe(1C)-C(10C)	68.1(2)
C(5C)-Fe(1C)-C(10C)	109.1(2)
C(8C)-Fe(1C)-C(10C)	67.8(2)
C(3C)-Fe(1C)-C(10C)	158.3(2)
C(1C)-Fe(1C)-C(4C)	68.8(2)
C(2C)-Fe(1C)-C(4C)	67.1(2)
C(7C)-Fe(1C)-C(4C)	160.53(18)
C(5C)-Fe(1C)-C(4C)	39.99(18)
C(8C)-Fe(1C)-C(4C)	124.52(18)
C(3C)-Fe(1C)-C(4C)	40.33(18)
C(10C)-Fe(1C)-C(4C)	123.3(2)
C(1C)-Fe(1C)-C(6C)	105.4(2)
C(2C)-Fe(1C)-C(6C)	123.3(2)
C(7C)-Fe(1C)-C(6C)	40.81(19)
C(5C)-Fe(1C)-C(6C)	122.0(2)
C(8C)-Fe(1C)-C(6C)	69.01(19)
C(3C)-Fe(1C)-C(6C)	159.4(2)
C(10C)-Fe(1C)-C(6C)	41.02(18)
C(4C)-Fe(1C)-C(6C)	158.0(2)
C(1C)-Fe(1C)-C(9C)	160.3(2)
C(2C)-Fe(1C)-C(9C)	157.74(19)
C(7C)-Fe(1C)-C(9C)	68.10(19)

C(5C)-Fe(1C)-C(9C)	125.3(2)
C(8C)-Fe(1C)-C(9C)	40.17(17)
C(3C)-Fe(1C)-C(9C)	123.03(19)
C(10C)-Fe(1C)-C(9C)	40.01(18)
C(4C)-Fe(1C)-C(9C)	109.4(2)
C(6C)-Fe(1C)-C(9C)	68.59(19)
C(5C)-C(1C)-C(2C)	105.0(5)
C(5C)-C(1C)-Fe(1C)	70.4(3)
C(2C)-C(1C)-Fe(1C)	69.8(3)
C(5C)-C(1C)-H(1C)	127.4
C(2C)-C(1C)-H(1C)	127.4
Fe(1C)-C(1C)-H(1C)	127.4
C(3C)-C(2C)-C(1C)	110.3(5)
C(3C)-C(2C)-Fe(1C)	70.9(3)
C(1C)-C(2C)-Fe(1C)	69.0(3)
C(3C)-C(2C)-H(2C)	124.8
C(1C)-C(2C)-H(2C)	124.8
Fe(1C)-C(2C)-H(2C)	124.8
C(2C)-C(3C)-C(4C)	107.1(5)
C(2C)-C(3C)-Fe(1C)	69.2(3)
C(4C)-C(3C)-Fe(1C)	70.0(3)
C(2C)-C(3C)-H(3C)	126.4
C(4C)-C(3C)-H(3C)	126.4
Fe(1C)-C(3C)-H(3C)	126.4
C(5C)-C(4C)-C(3C)	107.9(5)
C(5C)-C(4C)-Fe(1C)	69.6(3)
C(3C)-C(4C)-Fe(1C)	69.7(3)
C(5C)-C(4C)-H(4C)	126.1
C(3C)-C(4C)-H(4C)	126.1
Fe(1C)-C(4C)-H(4C)	126.1
C(4C)-C(5C)-C(1C)	109.6(5)
C(4C)-C(5C)-Fe(1C)	70.5(3)
C(1C)-C(5C)-Fe(1C)	68.7(3)
C(4C)-C(5C)-H(5C)	125.2
C(1C)-C(5C)-H(5C)	125.2
Fe(1C)-C(5C)-H(5C)	125.2
C(7C)-C(6C)-C(10C)	105.8(4)
C(7C)-C(6C)-C(11C)	127.4(5)
C(10C)-C(6C)-C(11C)	126.7(5)
C(7C)-C(6C)-Fe(1C)	68.6(3)
C(10C)-C(6C)-Fe(1C)	69.3(3)
C(11C)-C(6C)-Fe(1C)	126.6(4)
C(6C)-C(7C)-C(8C)	109.1(4)
C(6C)-C(7C)-Fe(1C)	70.6(3)
C(8C)-C(7C)-Fe(1C)	70.0(3)
C(6C)-C(7C)-H(7C)	125.5
C(8C)-C(7C)-H(7C)	125.5
Fe(1C)-C(7C)-H(7C)	125.5
C(9C)-C(8C)-C(7C)	107.6(4)
C(9C)-C(8C)-Fe(1C)	70.4(3)
C(7C)-C(8C)-Fe(1C)	68.9(3)
C(9C)-C(8C)-H(8C)	126.2
C(7C)-C(8C)-H(8C)	126.2
Fe(1C)-C(8C)-H(8C)	126.2
C(10C)-C(9C)-C(8C)	108.5(4)
C(10C)-C(9C)-Fe(1C)	69.8(3)

C(8C)-C(9C)-Fe(1C) 69.4(3)
C(10C)-C(9C)-H(9C) 125.8
C(8C)-C(9C)-H(9C) 125.8
Fe(1C)-C(9C)-H(9C) 125.8
C(9C)-C(10C)-C(6C) 109.1(5)
C(9C)-C(10C)-Fe(1C) 70.2(3)
C(6C)-C(10C)-Fe(1C) 69.7(3)
C(9C)-C(10C)-H(10C) 125.4
C(6C)-C(10C)-H(10C) 125.4
Fe(1C)-C(10C)-H(10C) 125.4
C(16C)-C(11C)-C(12C) 117.9(5)
C(16C)-C(11C)-C(6C) 121.3(5)
C(12C)-C(11C)-C(6C) 120.5(5)
C(13C)-C(12C)-C(11C) 120.2(5)
C(13C)-C(12C)-H(12C) 119.9
C(11C)-C(12C)-H(12C) 119.9
C(12C)-C(13C)-C(14C) 122.7(5)
C(12C)-C(13C)-H(13C) 118.6
C(14C)-C(13C)-H(13C) 118.6
C(15C)-C(14C)-C(13C) 115.5(5)
C(15C)-C(14C)-C(17C) 123.2(5)
C(13C)-C(14C)-C(17C) 121.2(5)
C(16C)-C(15C)-C(14C) 122.9(5)
C(16C)-C(15C)-H(15C) 118.5
C(14C)-C(15C)-H(15C) 118.5
C(15C)-C(16C)-C(11C) 120.7(5)
C(15C)-C(16C)-H(16C) 119.7
C(11C)-C(16C)-H(16C) 119.7
C(23C)-C(17C)-C(14C) 112.8(5)
C(23C)-C(17C)-C(18C) 117.6(5)
C(14C)-C(17C)-C(18C) 109.8(5)
C(23C)-C(17C)-H(17C) 105.1
C(14C)-C(17C)-H(17C) 105.1
C(18C)-C(17C)-H(17C) 105.1
C(19C)-C(18C)-C(22C) 103.1(4)
C(19C)-C(18C)-C(17C) 114.9(5)
C(22C)-C(18C)-C(17C) 114.5(5)
C(19C)-C(18C)-H(18C) 108.0
C(22C)-C(18C)-H(18C) 108.0
C(17C)-C(18C)-H(18C) 108.0
C(18C)-C(19C)-C(20C) 105.4(4)
C(18C)-C(19C)-H(19E) 110.7
C(20C)-C(19C)-H(19E) 110.7
C(18C)-C(19C)-H(19F) 110.7
C(20C)-C(19C)-H(19F) 110.7
H(19E)-C(19C)-H(19F) 108.8
C(21C)-C(20C)-C(19C) 105.5(4)
C(21C)-C(20C)-H(20E) 110.6
C(19C)-C(20C)-H(20E) 110.6
C(21C)-C(20C)-H(20F) 110.6
C(19C)-C(20C)-H(20F) 110.6
H(20E)-C(20C)-H(20F) 108.8
C(22C)-C(21C)-C(20C) 107.3(5)
C(22C)-C(21C)-H(21E) 110.3
C(20C)-C(21C)-H(21E) 110.3
C(22C)-C(21C)-H(21F) 110.3

C(20C)-C(21C)-H(21F)	110.3
H(21E)-C(21C)-H(21F)	108.5
C(21C)-C(22C)-C(18C)	103.6(5)
C(21C)-C(22C)-H(22E)	111.0
C(18C)-C(22C)-H(22E)	111.0
C(21C)-C(22C)-H(22F)	111.0
C(18C)-C(22C)-H(22F)	111.0
H(22E)-C(22C)-H(22F)	109.0
C(17C)-C(23C)-H(23G)	109.5
C(17C)-C(23C)-H(23H)	109.5
H(23G)-C(23C)-H(23H)	109.5
C(17C)-C(23C)-H(23I)	109.5
H(23G)-C(23C)-H(23I)	109.5
H(23H)-C(23C)-H(23I)	109.5
C(7D)-Fe(1D)-C(1D)	122.8(3)
C(7D)-Fe(1D)-C(4D)	158.7(2)
C(1D)-Fe(1D)-C(4D)	67.7(2)
C(7D)-Fe(1D)-C(2D)	107.7(3)
C(1D)-Fe(1D)-C(2D)	40.5(2)
C(4D)-Fe(1D)-C(2D)	67.2(3)
C(7D)-Fe(1D)-C(5D)	159.3(2)
C(1D)-Fe(1D)-C(5D)	40.6(2)
C(4D)-Fe(1D)-C(5D)	40.1(2)
C(2D)-Fe(1D)-C(5D)	67.8(2)
C(7D)-Fe(1D)-C(8D)	40.4(2)
C(1D)-Fe(1D)-C(8D)	158.6(3)
C(4D)-Fe(1D)-C(8D)	123.5(2)
C(2D)-Fe(1D)-C(8D)	122.9(3)
C(5D)-Fe(1D)-C(8D)	159.2(2)
C(7D)-Fe(1D)-C(3D)	122.6(3)
C(1D)-Fe(1D)-C(3D)	67.6(3)
C(4D)-Fe(1D)-C(3D)	40.3(2)
C(2D)-Fe(1D)-C(3D)	39.6(2)
C(5D)-Fe(1D)-C(3D)	67.7(2)
C(8D)-Fe(1D)-C(3D)	108.0(2)
C(7D)-Fe(1D)-C(9D)	68.1(2)
C(1D)-Fe(1D)-C(9D)	159.4(3)
C(4D)-Fe(1D)-C(9D)	108.8(2)
C(2D)-Fe(1D)-C(9D)	158.8(3)
C(5D)-Fe(1D)-C(9D)	123.5(3)
C(8D)-Fe(1D)-C(9D)	40.5(2)
C(3D)-Fe(1D)-C(9D)	123.8(3)
C(7D)-Fe(1D)-C(6D)	40.9(2)
C(1D)-Fe(1D)-C(6D)	107.1(2)
C(4D)-Fe(1D)-C(6D)	159.5(3)
C(2D)-Fe(1D)-C(6D)	122.7(3)
C(5D)-Fe(1D)-C(6D)	123.1(2)
C(8D)-Fe(1D)-C(6D)	68.6(2)
C(3D)-Fe(1D)-C(6D)	158.1(3)
C(9D)-Fe(1D)-C(6D)	68.6(2)
C(7D)-Fe(1D)-C(10D)	67.8(2)
C(1D)-Fe(1D)-C(10D)	123.7(3)
C(4D)-Fe(1D)-C(10D)	124.3(3)
C(2D)-Fe(1D)-C(10D)	159.4(3)
C(5D)-Fe(1D)-C(10D)	108.9(2)
C(8D)-Fe(1D)-C(10D)	67.6(2)

C(3D)-Fe(1D)-C(10D)	159.8(3)
C(9D)-Fe(1D)-C(10D)	40.1(2)
C(6D)-Fe(1D)-C(10D)	40.7(2)
C(2D)-C(1D)-C(5D)	107.3(6)
C(2D)-C(1D)-Fe(1D)	69.9(3)
C(5D)-C(1D)-Fe(1D)	69.9(3)
C(2D)-C(1D)-H(1D)	126.3
C(5D)-C(1D)-H(1D)	126.3
Fe(1D)-C(1D)-H(1D)	126.3
C(3D)-C(2D)-C(1D)	108.9(6)
C(3D)-C(2D)-Fe(1D)	70.8(4)
C(1D)-C(2D)-Fe(1D)	69.6(3)
C(3D)-C(2D)-H(2D)	125.5
C(1D)-C(2D)-H(2D)	125.5
Fe(1D)-C(2D)-H(2D)	125.5
C(2D)-C(3D)-C(4D)	107.5(6)
C(2D)-C(3D)-Fe(1D)	69.6(4)
C(4D)-C(3D)-Fe(1D)	69.1(3)
C(2D)-C(3D)-H(3D)	126.3
C(4D)-C(3D)-H(3D)	126.3
Fe(1D)-C(3D)-H(3D)	126.3
C(5D)-C(4D)-C(3D)	108.8(6)
C(5D)-C(4D)-Fe(1D)	70.1(3)
C(3D)-C(4D)-Fe(1D)	70.6(3)
C(5D)-C(4D)-H(4D)	125.6
C(3D)-C(4D)-H(4D)	125.6
Fe(1D)-C(4D)-H(4D)	125.6
C(4D)-C(5D)-C(1D)	107.5(6)
C(4D)-C(5D)-Fe(1D)	69.8(3)
C(1D)-C(5D)-Fe(1D)	69.5(3)
C(4D)-C(5D)-H(5D)	126.2
C(1D)-C(5D)-H(5D)	126.2
Fe(1D)-C(5D)-H(5D)	126.2
C(7D)-C(6D)-C(10D)	105.8(5)
C(7D)-C(6D)-C(11D)	126.4(6)
C(10D)-C(6D)-C(11D)	127.8(6)
C(7D)-C(6D)-Fe(1D)	68.4(3)
C(10D)-C(6D)-Fe(1D)	69.8(3)
C(11D)-C(6D)-Fe(1D)	128.1(4)
C(8D)-C(7D)-C(6D)	109.3(6)
C(8D)-C(7D)-Fe(1D)	70.1(3)
C(6D)-C(7D)-Fe(1D)	70.7(3)
C(8D)-C(7D)-H(7D)	125.4
C(6D)-C(7D)-H(7D)	125.4
Fe(1D)-C(7D)-H(7D)	125.4
C(7D)-C(8D)-C(9D)	108.3(5)
C(7D)-C(8D)-Fe(1D)	69.5(3)
C(9D)-C(8D)-Fe(1D)	70.4(3)
C(7D)-C(8D)-H(8D)	125.9
C(9D)-C(8D)-H(8D)	125.9
Fe(1D)-C(8D)-H(8D)	125.9
C(10D)-C(9D)-C(8D)	107.4(5)
C(10D)-C(9D)-Fe(1D)	70.1(3)
C(8D)-C(9D)-Fe(1D)	69.0(3)
C(10D)-C(9D)-H(9D)	126.3
C(8D)-C(9D)-H(9D)	126.3

Fe(1D)-C(9D)-H(9D) 126.3
C(9D)-C(10D)-C(6D) 109.2(6)
C(9D)-C(10D)-Fe(1D) 69.7(3)
C(6D)-C(10D)-Fe(1D) 69.6(3)
C(9D)-C(10D)-H(10D) 125.4
C(6D)-C(10D)-H(10D) 125.4
Fe(1D)-C(10D)-H(10D)125.4
C(12D)-C(11D)-C(16D)117.8(6)
C(12D)-C(11D)-C(6D) 121.8(6)
C(16D)-C(11D)-C(6D) 120.4(6)
C(13D)-C(12D)-C(11D)121.1(6)
C(13D)-C(12D)-H(12D)119.5
C(11D)-C(12D)-H(12D)119.5
C(12D)-C(13D)-C(14D)121.9(6)
C(12D)-C(13D)-H(13D)119.1
C(14D)-C(13D)-H(13D)119.1
C(15D)-C(14D)-C(13D)116.6(6)
C(15D)-C(14D)-C(17D)122.0(6)
C(13D)-C(14D)-C(17D)121.4(6)
C(14D)-C(15D)-C(16D)123.6(6)
C(14D)-C(15D)-H(15D)118.2
C(16D)-C(15D)-H(15D)118.2
C(11D)-C(16D)-C(15D)119.0(6)
C(11D)-C(16D)-H(16D)120.5
C(15D)-C(16D)-H(16D)120.5
C(18D)-C(17D)-C(23D)116.2(5)
C(18D)-C(17D)-C(14D)114.0(5)
C(23D)-C(17D)-C(14D)109.8(5)
C(18D)-C(17D)-H(17D)105.2
C(23D)-C(17D)-H(17D)105.2
C(14D)-C(17D)-H(17D)105.2
C(17D)-C(18D)-C(19D)117.9(5)
C(17D)-C(18D)-C(22D)113.6(4)
C(19D)-C(18D)-C(22D)105.3(4)
C(17D)-C(18D)-H(18D)106.4
C(19D)-C(18D)-H(18D)106.4
C(22D)-C(18D)-H(18D)106.4
C(20D)-C(19D)-C(18D)106.6(5)
C(20D)-C(19D)-H(19G)110.4
C(18D)-C(19D)-H(19G)110.4
C(20D)-C(19D)-H(19H)110.4
C(18D)-C(19D)-H(19H)110.4
H(19G)-C(19D)-H(19H)108.6
C(19D)-C(20D)-C(21D)113.1(6)
C(19D)-C(20D)-H(20G)109.0
C(21D)-C(20D)-H(20G)109.0
C(19D)-C(20D)-H(20H)109.0
C(21D)-C(20D)-H(20H)109.0
H(20G)-C(20D)-H(20H)107.8
C(20D)-C(21D)-C(22D)106.6(4)
C(20D)-C(21D)-H(21G)110.4
C(22D)-C(21D)-H(21G)110.4
C(20D)-C(21D)-H(21H)110.4
C(22D)-C(21D)-H(21H)110.4
H(21G)-C(21D)-H(21H)108.6
C(21D)-C(22D)-C(18D)106.4(4)

C(21D)-C(22D)-H(22G)110.4
C(18D)-C(22D)-H(22G)110.4
C(21D)-C(22D)-H(22H)110.4
C(18D)-C(22D)-H(22H)110.4
H(22G)-C(22D)-H(22H)108.6
C(17D)-C(23D)-H(23J) 109.5
C(17D)-C(23D)-H(23K)109.5
H(23J)-C(23D)-H(23K) 109.5
C(17D)-C(23D)-H(23L)109.5
H(23J)-C(23D)-H(23L) 109.5
H(23K)-C(23D)-H(23L)109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for cjc01. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

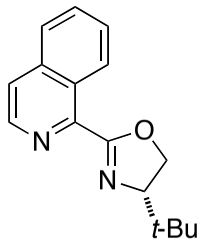
U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1A)372(5)	260(6)	229(5)	25(4)	9(4)	5(4)
C(1A)460(30)	250(30)	160(20)	80(19)	20(20)	-130(20)
C(2A)290(30)	190(30)	370(30)	0(30)	100(30)	40(30)
C(3A)280(30)	220(30)	440(30)	40(20)	-40(20)	-90(20)
C(4A)470(30)	240(30)	390(30)	-80(20)	70(30)	-170(20)
C(5A)500(40)	150(30)	430(40)	-10(30)	150(30)	-50(30)
C(6A)240(30)	290(40)	240(30)	-40(30)	60(30)	-20(30)
C(7A)320(30)	140(20)	380(30)	-20(20)	100(20)	-60(20)
C(8A)370(30)	240(30)	440(30)	190(20)	-50(20)	-130(20)
C(9A)480(40)	410(40)	310(40)	-160(30)	200(30)	-190(30)
C(10A)380(30)	300(30)	360(30)	20(20)	40(20)	50(20)
C(11A)310(40)	270(40)	240(30)	80(30)	40(30)	40(30)
C(12A)520(40)	280(30)	190(30)	-90(20)	-40(30)	-20(30)
C(13A)580(40)	270(30)	340(40)	-90(30)	-10(30)	130(30)
C(14A)640(40)	340(30)	130(30)	20(20)	-40(30)	70(30)
C(15A)640(50)	330(40)	180(30)	-130(30)	60(30)	-180(30)
C(16A)600(40)	200(30)	420(30)	30(20)	100(30)	70(20)
C(17A)780(50)	380(40)	300(30)	-70(30)	-60(30)	110(30)
C(18A)640(50)	570(40)	240(30)	0(30)	0(30)	200(40)
C(19A)730(50)	1620(80)	320(40)	-150(40)	-130(30)	760(50)
C(20A)890(60)	1260(70)	470(40)	80(40)	420(40)	-50(60)
C(21A)560(50)	2430(110)	330(40)	290(50)	-30(40)	90(60)
C(22A)910(50)	870(50)	370(30)	-10(40)	-150(30)	270(50)
C(23A)820(40)	510(30)	250(30)	-40(20)	-70(30)	-120(30)
Fe(1B)79(4)	36(4)	199(4)	-9(3)	51(3)	27(3)
C(1B)163(14)	154(14)	152(14)	-19(9)	27(9)	22(9)
C(2B)140(30)	70(30)	320(30)	40(20)	90(20)	-30(20)
C(3B)144(14)	150(14)	171(14)	-9(9)	0(9)	15(9)
C(4B)200(15)	174(15)	195(15)	11(9)	21(9)	28(9)
C(5B)185(15)	158(15)	193(15)	-12(9)	15(9)	-3(9)
C(6B)140(30)	50(30)	160(30)	-10(20)	50(20)	20(20)
C(7B) 90(13)	77(13)	105(13)	-7(9)	9(9)	10(9)
C(8B)145(14)	134(14)	159(14)	-21(9)	17(9)	11(9)
C(9B)160(30)	110(30)	230(30)	10(20)	70(20)	80(20)
C(10B)70(20)	230(30)	110(30)	-20(20)	40(20)	20(20)
C(11B)80(30)	150(30)	140(30)	60(20)	40(20)	60(20)
C(12B)210(30)	110(30)	180(30)	-30(20)	20(20)	-50(20)
C(13B)270(30)	90(20)	240(30)	40(20)	-40(20)	0(20)
C(14B)380(30)	150(30)	210(30)	-130(20)	-30(20)	-60(30)
C(15B)300(30)	80(30)	130(30)	20(20)	-50(20)	50(20)
C(16B)230(30)	100(30)	140(30)	-60(20)	-30(20)	-10(20)
C(17B)270(30)	220(30)	280(30)	-70(20)	0(20)	110(20)
C(18B)230(20)	230(20)	250(20)	-46(19)	-38(17)	1(19)
C(19B)420(40)	490(50)	280(40)	-120(30)	50(30)	-10(40)
C(20B)330(30)	780(40)	580(40)	-460(30)	100(30)	-80(30)
C(21B)250(30)	1470(60)	680(40)	-480(50)	-20(30)	170(40)
C(22B)270(30)	620(40)	350(30)	-150(30)	-40(20)	70(30)
C(23B)330(30)	780(40)	220(20)	-180(30)	-10(20)	-50(30)
Fe(1C)80(4)	43(4)	188(4)	-8(3)	53(3)	-15(3)
C(1C)219(15)	194(15)	221(15)	14(9)	19(9)	-12(9)
C(2C)170(30)	40(30)	320(30)	20(20)	60(20)	10(20)

C(3C)145(14)	137(14)	143(14)	-8(9)	8(9)	-26(9)
C(4C)127(14)	131(14)	165(14)	11(9)	10(9)	-10(9)
C(5C)210(30)	90(30)	210(30)	-30(20)	120(20)	-120(20)
C(6C) 90(30)	70(30)	220(30)	20(20)	20(20)	-40(20)
C(7C) 88(14)	101(14)	96(14)	-13(9)	21(9)	-5(9)
C(8C) 80(30)	130(30)	120(30)	90(20)	-20(20)	0(20)
C(9C)113(13)	105(13)	115(13)	17(9)	11(9)	-11(9)
C(10C)140(14)	124(14)	150(14)	-4(9)	13(9)	-3(9)
C(11C)130(30)	80(30)	170(30)	-70(20)	50(20)	-10(20)
C(12C)137(14)	117(14)	119(14)	-13(9)	12(9)	5(9)
C(13C)290(30)	120(30)	290(30)	40(20)	-10(30)	90(20)
C(14C)200(30)	220(30)	180(30)	-90(20)	-30(20)	-20(20)
C(15C)350(30)	140(30)	330(30)	30(20)	-120(30)	100(20)
C(16C)240(30)	170(30)	270(30)	-100(20)	-30(20)	110(20)
C(17C)320(30)	400(40)	250(30)	0(20)	-70(20)	60(30)
C(18C)280(30)	440(40)	180(30)	0(20)	-60(20)	130(20)
C(19C)320(30)	520(40)	280(30)	-60(20)	-40(20)	60(30)
C(20C)220(30)	330(30)	380(30)	50(20)	30(20)	60(20)
C(21C)250(30)	400(30)	750(40)	-240(30)	-80(30)	-80(20)
C(22C)270(30)	670(40)	510(40)	-310(30)	70(30)	-70(30)
C(23C)560(40)	750(40)	480(30)	250(30)	-260(30)	-230(30)
Fe(1D)357(5)	270(6)	234(5)	-19(4)	-26(4)	16(4)
C(1D)370(30)	230(30)	490(30)	-200(20)	-10(30)	60(20)
C(2D)460(40)	80(20)	760(40)	50(20)	230(30)	80(20)
C(3D)570(40)	360(30)	280(30)	80(20)	40(30)	280(30)
C(4D)250(30)	320(30)	580(40)	-160(30)	-120(30)	60(20)
C(5D)340(30)	320(40)	250(30)	-10(30)	90(30)	140(30)
C(6D)230(30)	260(30)	280(40)	-30(30)	-20(30)	80(30)
C(7D)310(30)	220(40)	390(40)	20(30)	50(30)	50(30)
C(8D)420(40)	400(40)	110(30)	-60(30)	-40(30)	110(30)
C(9D)350(30)	150(30)	490(30)	-130(20)	-80(20)	110(20)
C(10D)440(30)	140(20)	510(30)	10(20)	70(20)	150(20)
C(11D)280(30)	300(40)	260(30)	-110(30)	30(30)	-30(30)
C(12D)460(40)	320(40)	380(40)	80(30)	90(30)	50(30)
C(13D)370(40)	670(50)	310(40)	170(30)	0(30)	10(30)
C(14D)130(30)	610(40)	210(30)	100(30)	-20(20)	0(30)
C(15D)350(40)	540(50)	450(40)	-90(30)	-90(30)	-210(30)
C(16D)320(40)	520(50)	360(40)	150(30)	-70(30)	-50(30)
C(17D)270(40)	840(50)	240(30)	40(30)	-110(30)	-200(30)
C(18D)340(30)	490(30)	270(30)	-80(20)	-80(20)	90(20)
C(19D)340(40)	710(60)	670(50)	-320(50)	190(40)	-140(40)
C(20D)280(40)	3330(140)	1790(90)	-2210(100)	-430(50)	500(60)
C(21D)390(30)	770(40)	330(30)	-60(30)	-130(20)	100(30)
C(22D)360(30)	830(40)	300(30)	-160(30)	-120(20)	90(30)
C(23D)410(40)	3080(120)	420(40)	-840(60)	20(30)	160(60)

Table 5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for cjc01.

	x	y	z	U_{iso}
H(1A)	1107	380	397	35
H(2A)	1329	203	411	34
H(3A)	1393	210	470	38
H(4A)	1210	394	492	44
H(5A)	1027	496	447	42
H(7A)	1032	-14	421	33
H(8A)	1090	-7	480	42
H(9A)	906	180	501	47
H(10A)	741	286	456	41
H(12A)	741	369	404	40
H(13A)	608	416	357	48
H(15A)	676	42	330	46
H(16A)	804	-3	378	49
H(17A)	522	357	307	59
H(18A)	355	118	314	58
H(19A)	285	234	356	108
H(19B)	288	372	338	108
H(20A)	29	348	333	104
H(20B)	41	192	340	104
H(21A)	23	151	288	133
H(21B)	2	306	282	133
H(22A)	261	331	273	87
H(22B)	253	176	266	87
H(23A)	613	113	281	79
H(23B)	723	244	280	79
H(23C)	546	238	262	79
H(1B)	-80	1088	109	19
H(2B)	-314	919	96	21
H(3B)	-380	928	37	19
H(4B)	-183	1104	14	23
H(5B)	2	1203	58	21
H(7B)	-13	698	88	11
H(8B)	-92	694	30	17
H(9B)	87	868	3	20
H(10B)	276	984	46	16
H(12B)	283	1080	98	20
H(13B)	425	1134	144	24
H(15B)	390	758	172	21
H(16B)	247	704	126	19
H(17B)	519	1086	194	31
H(18B)	676	834	197	29
H(19C)	780	1063	166	48
H(19D)	777	914	154	48
H(20C)	1026	870	176	67
H(20D)	1047	1027	180	67
H(21C)	1042	996	229	96
H(21D)	986	846	225	96
H(22C)	775	1069	229	50
H(22D)	749	926	244	50
H(23D)	395	853	221	67
H(23E)	296	989	218	67

H(23F)	463	979	240	67
H(1C)	420	314	104	25
H(2C)	476	202	52	21
H(3C)	287	305	10	17
H(4C)	107	483	35	17
H(5C)	188	487	93	20
H(7C)	766	416	43	11
H(8C)	586	522	-2	14
H(9C)	407	704	22	13
H(10C)	475	713	80	17
H(12C)	681	708	122	15
H(13C)	823	672	169	28
H(15C)	928	302	143	33
H(16C)	791	336	96	27
H(17C)	960	539	205	39
H(18C)	1188	570	172	36
H(19E)	1251	464	232	45
H(19F)	1281	612	220	45
H(20E)	1537	561	204	37
H(20F)	1521	424	222	37
H(21E)	1489	466	160	57
H(21F)	1519	329	177	57
H(22E)	1245	292	181	58
H(22F)	1242	371	149	58
H(23G)	836	345	213	91
H(23H)	1023	334	226	91
H(23I)	970	266	195	91
H(1D)	561	595	392	44
H(2D)	495	496	444	51
H(3D)	689	599	485	48
H(4D)	875	766	459	47
H(5D)	799	763	401	36
H(7D)	221	724	454	37
H(8D)	412	832	495	37
H(9D)	598	1002	468	40
H(10D)	518	998	411	43
H(12D)	275	993	370	46
H(13D)	129	943	325	54
H(15D)	54	578	354	54
H(16D)	197	624	401	48
H(17D)	-40	806	294	54
H(18D)	-158	572	317	44
H(19G)	-307	684	348	68
H(19H)	-266	821	331	68
H(20G)	-499	816	308	218
H(20H)	-540	680	324	218
H(21G)	-505	714	265	61
H(21H)	-515	575	282	61
H(22G)	-237	695	261	60
H(22H)	-259	543	270	60
H(23J)	142	569	294	195
H(23K)	192	706	279	195
H(23L)	39	624	265	195



(*S*)-(*t*-Bu)-1-iQuinox (1)
^{1}H NMR (400 MHz, $CDCl_3$)

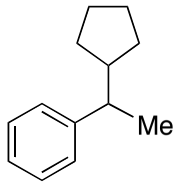
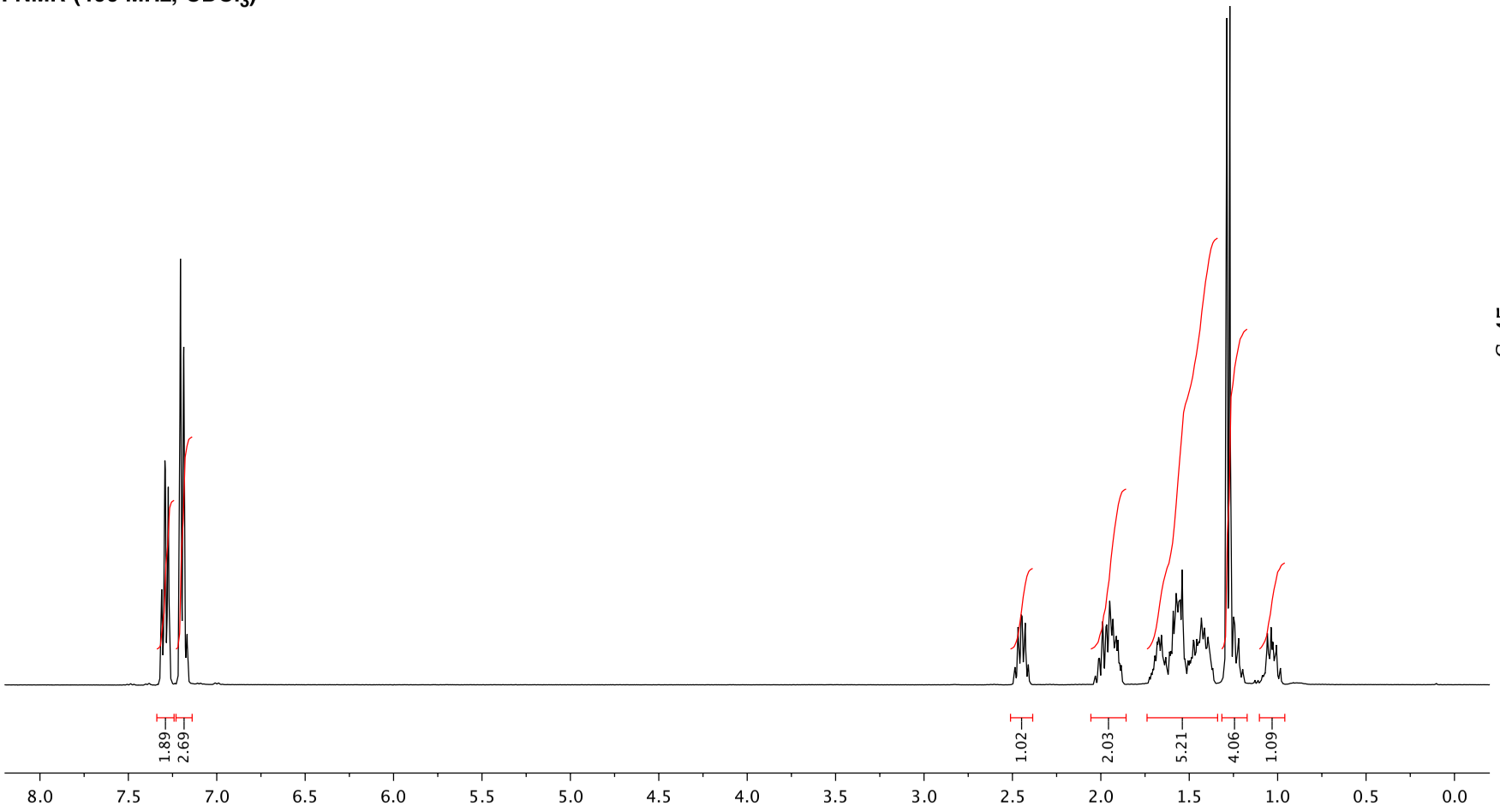


Table 2, entry 1
^{1}H NMR (400 MHz, $CDCl_3$)



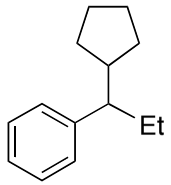
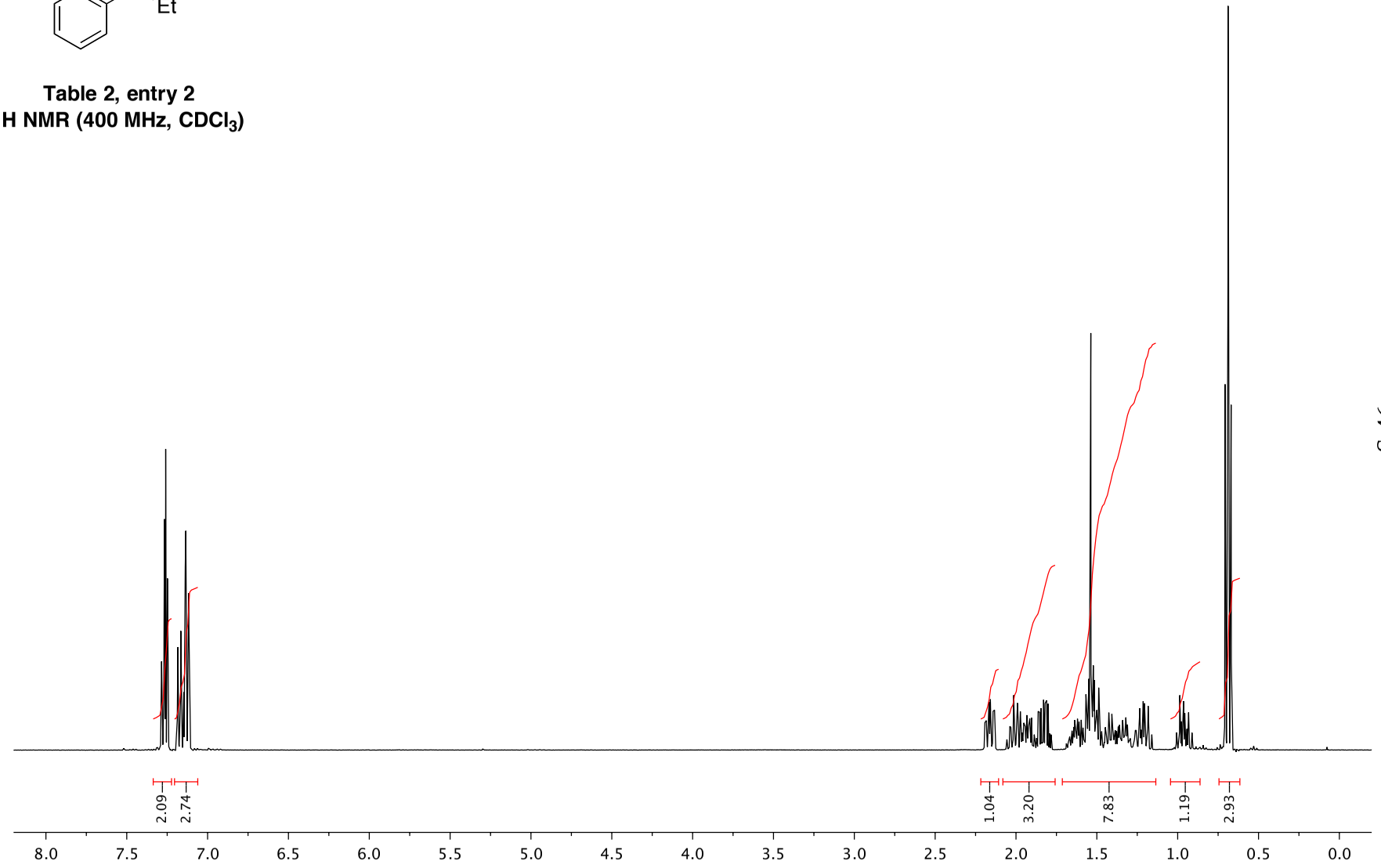


Table 2, entry 2
^{1}H NMR (400 MHz, $CDCl_3$)



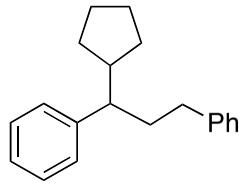
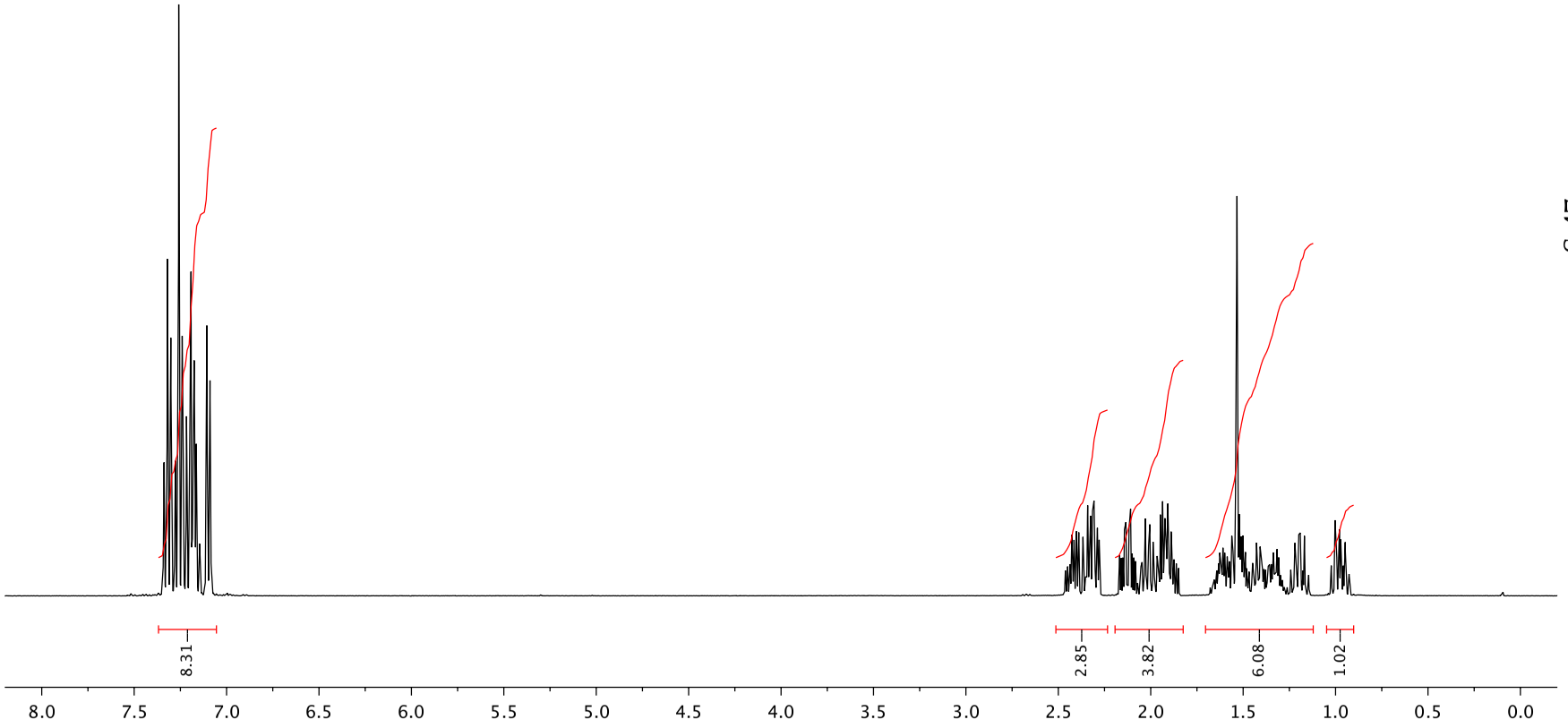


Table 2, entry 3
^{1}H NMR (400 MHz, $CDCl_3$)



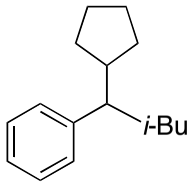
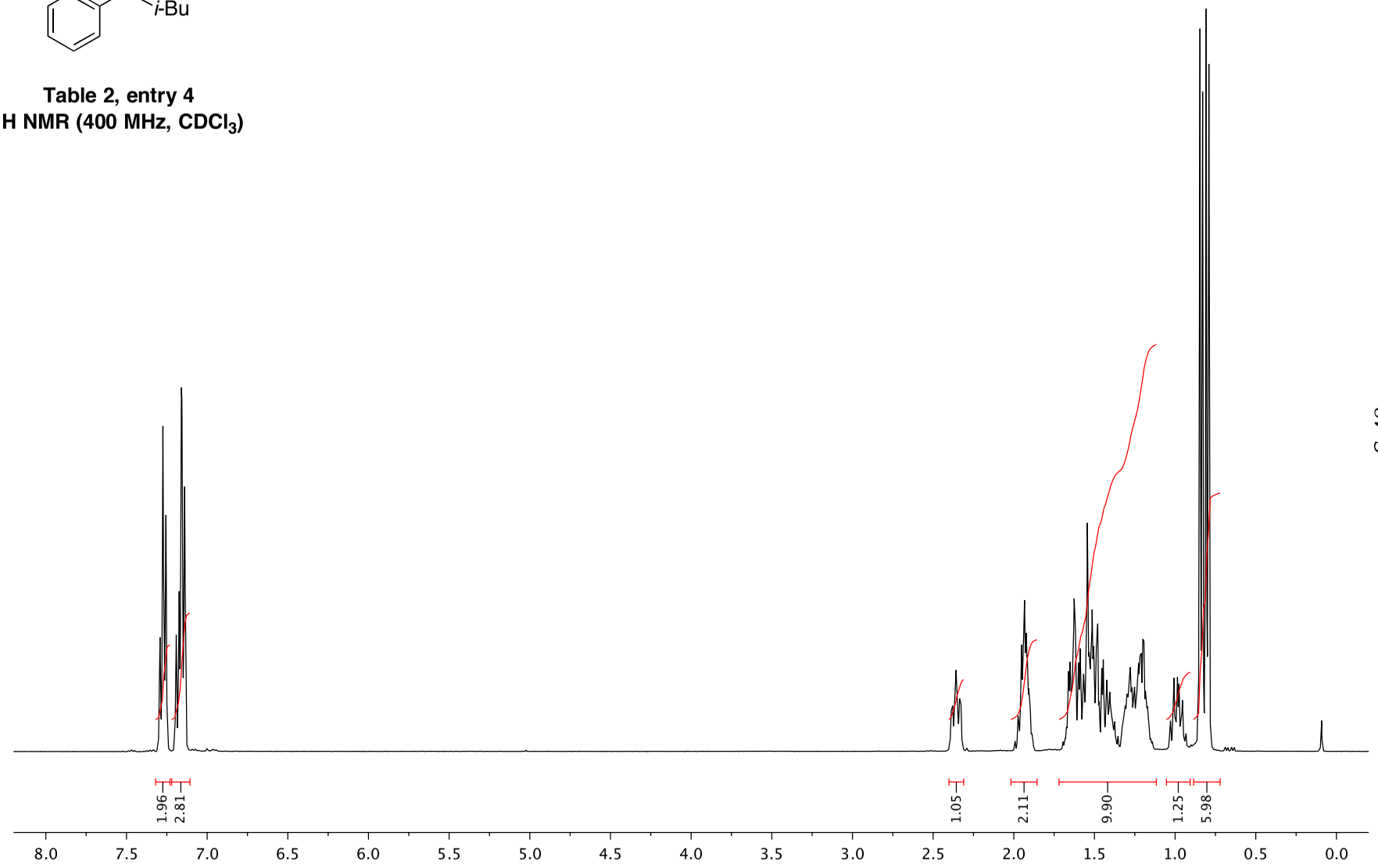


Table 2, entry 4
^{1}H NMR (400 MHz, $CDCl_3$)



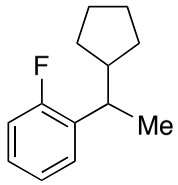
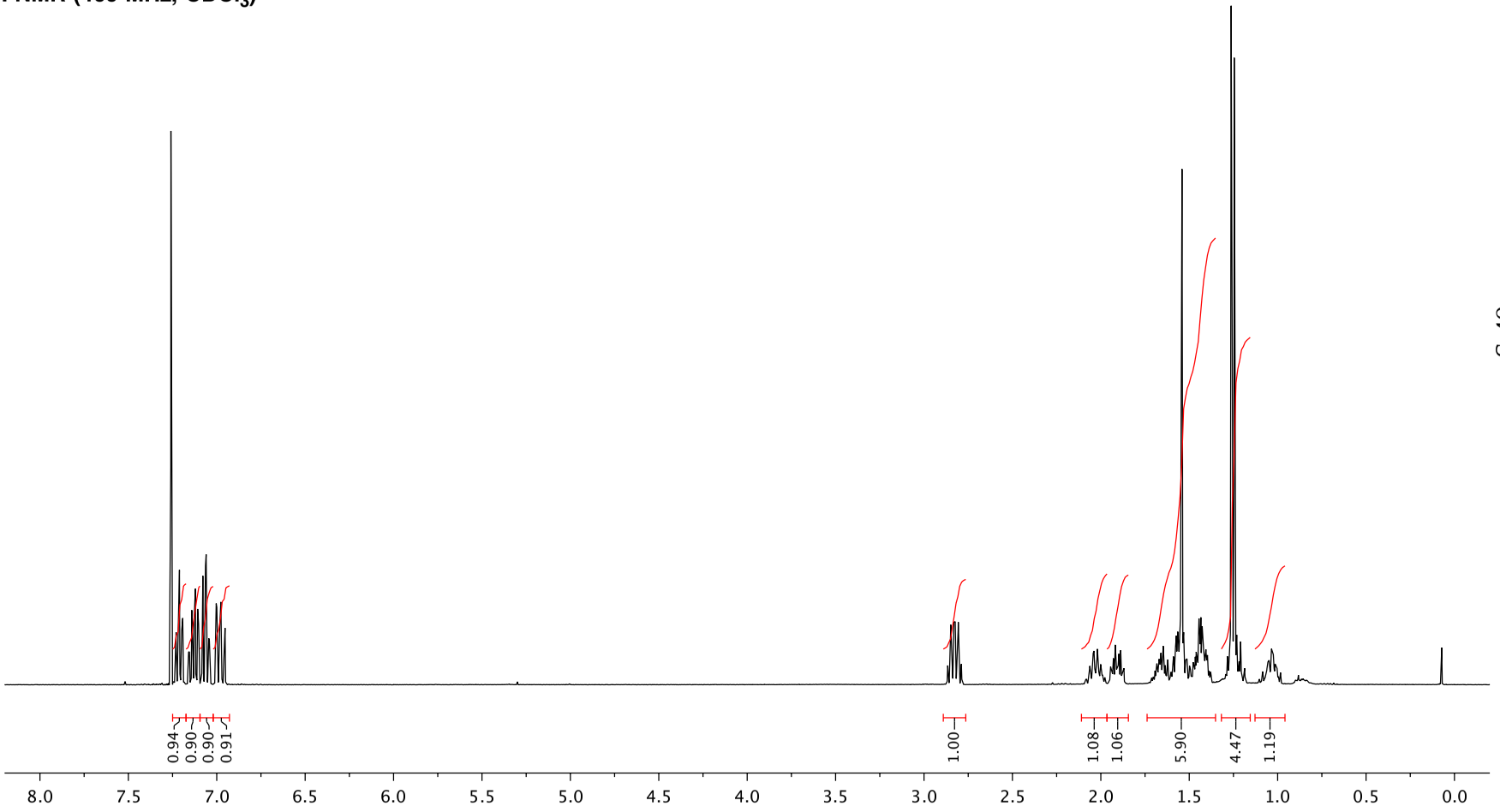


Table 2, entry 5
^{1}H NMR (400 MHz, $CDCl_3$)



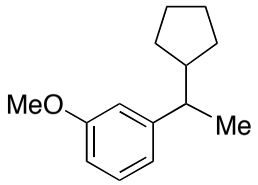
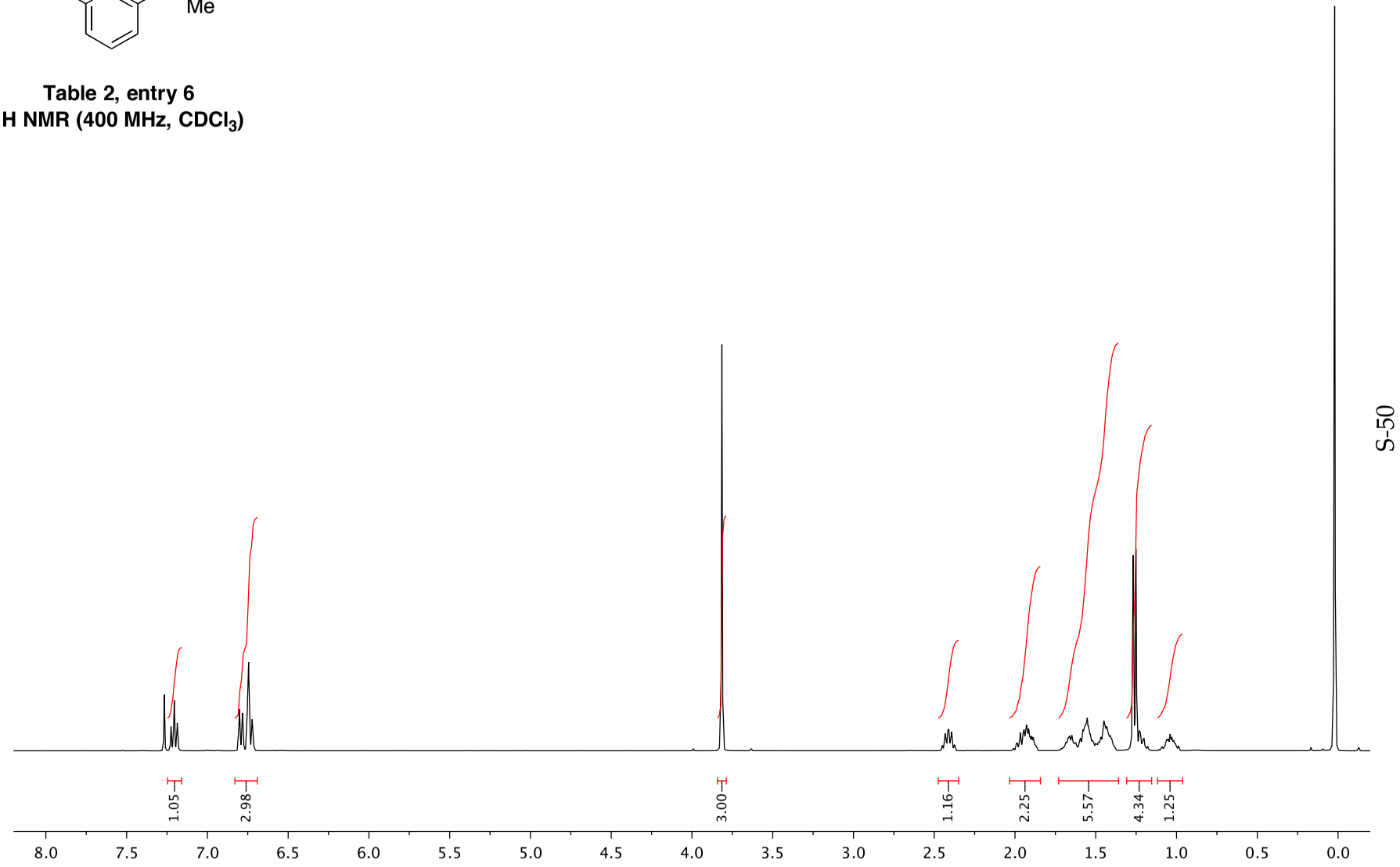


Table 2, entry 6
^{1}H NMR (400 MHz, $CDCl_3$)



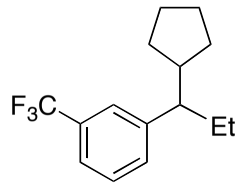


Table 2, entry 7
^{1}H NMR (400 MHz, $CDCl_3$)

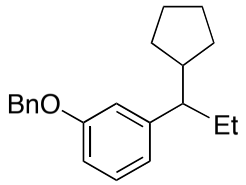


Table 2, entry 8
^{1}H NMR (400 MHz, $CDCl_3$)

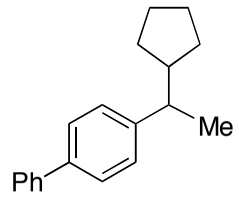
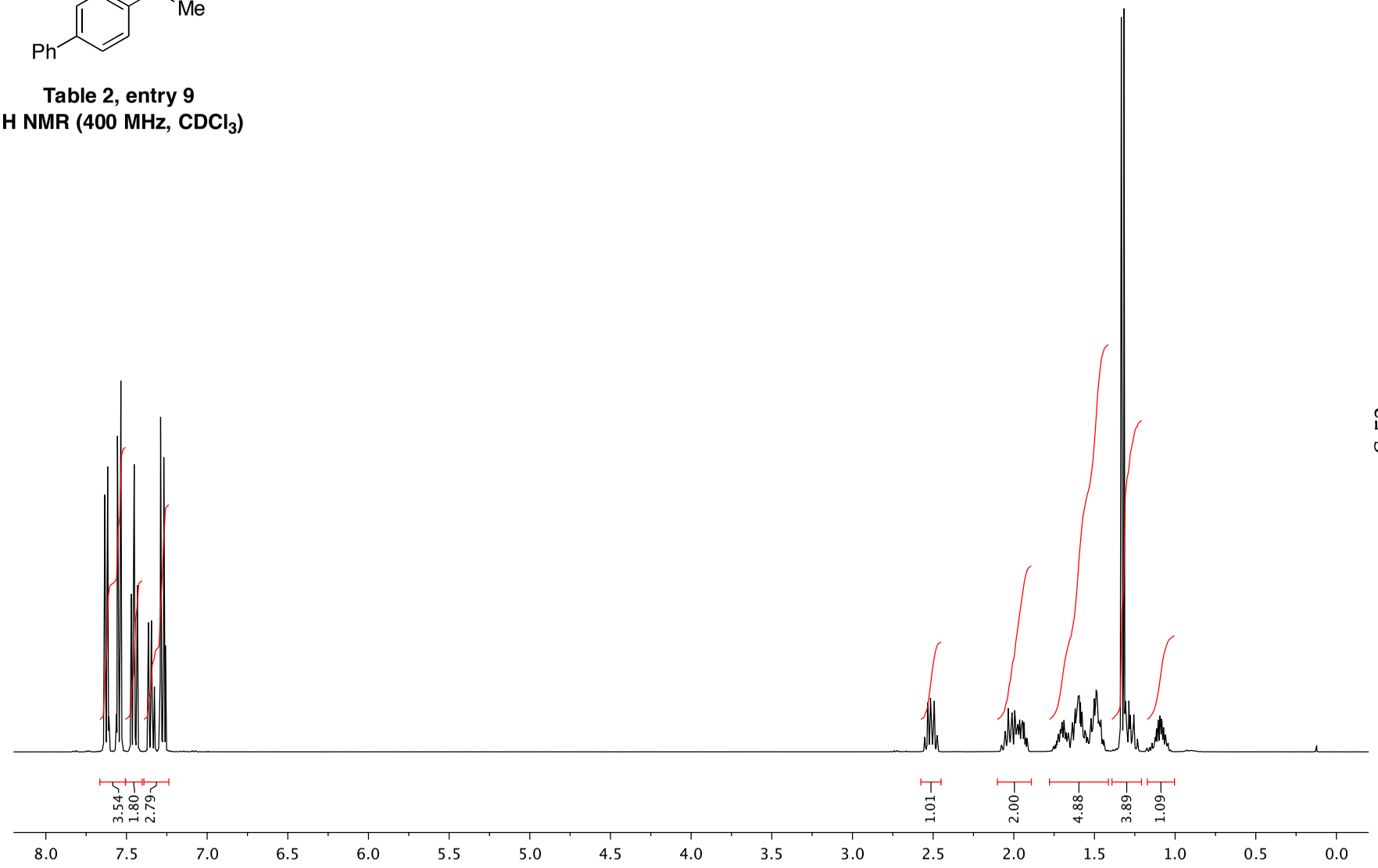


Table 2, entry 9
^{1}H NMR (400 MHz, $CDCl_3$)



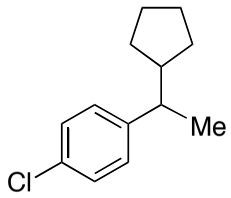
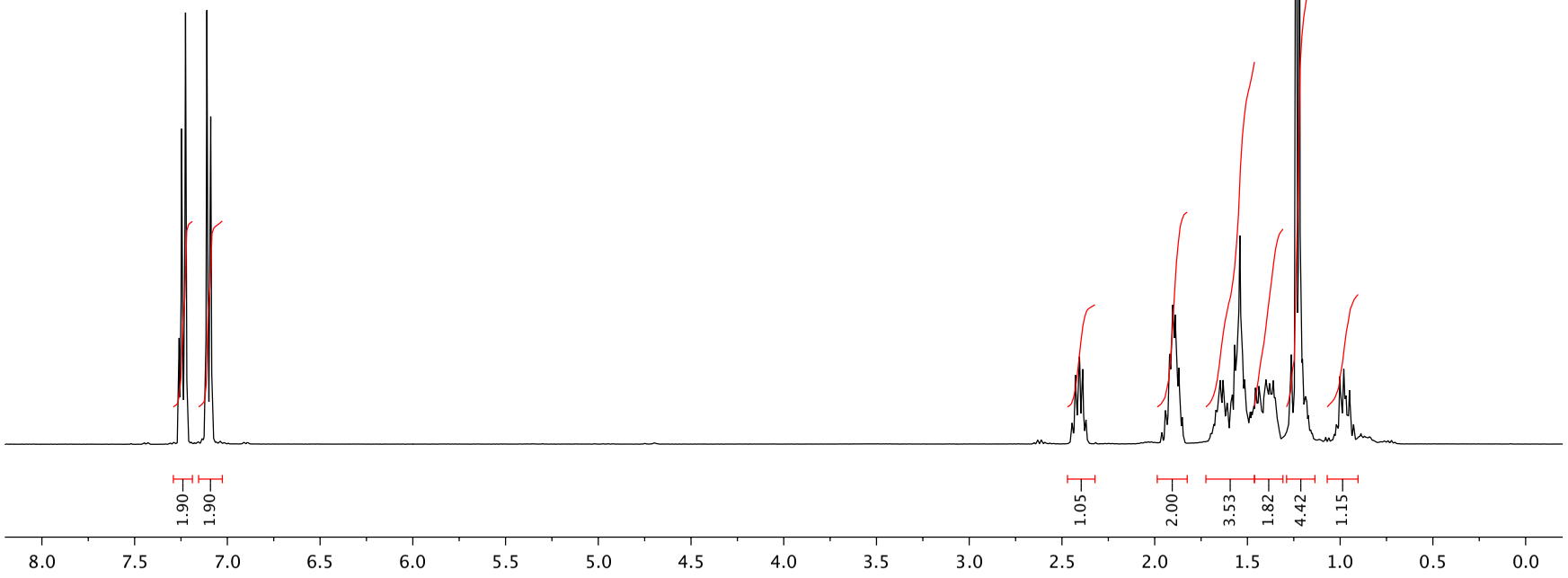


Table 2, entry 10
^{1}H NMR (400 MHz, $CDCl_3$)



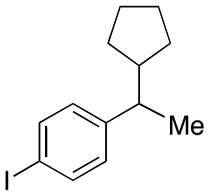
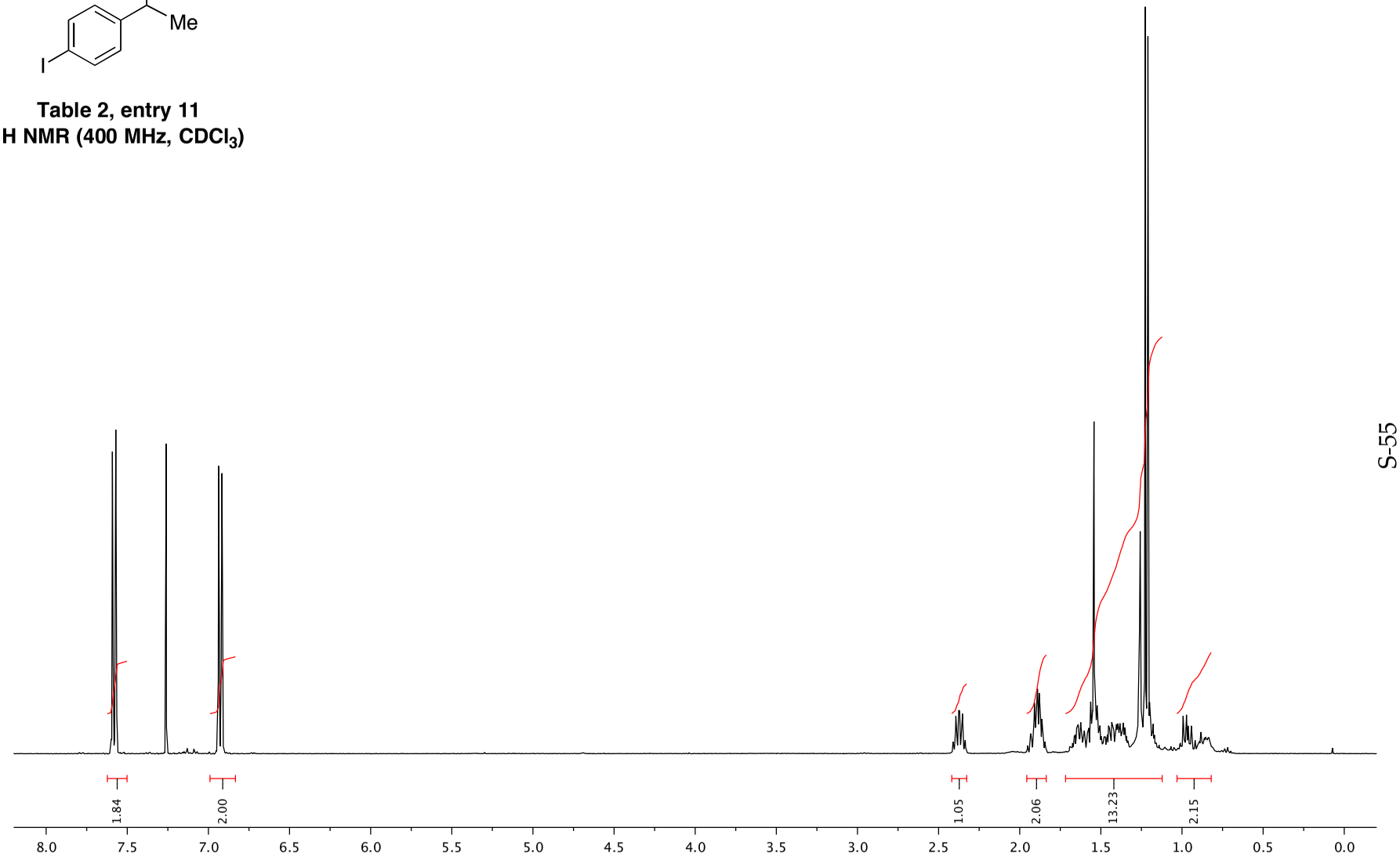


Table 2, entry 11
^{1}H NMR (400 MHz, $CDCl_3$)



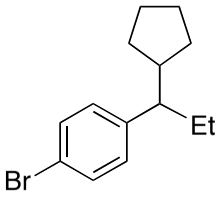
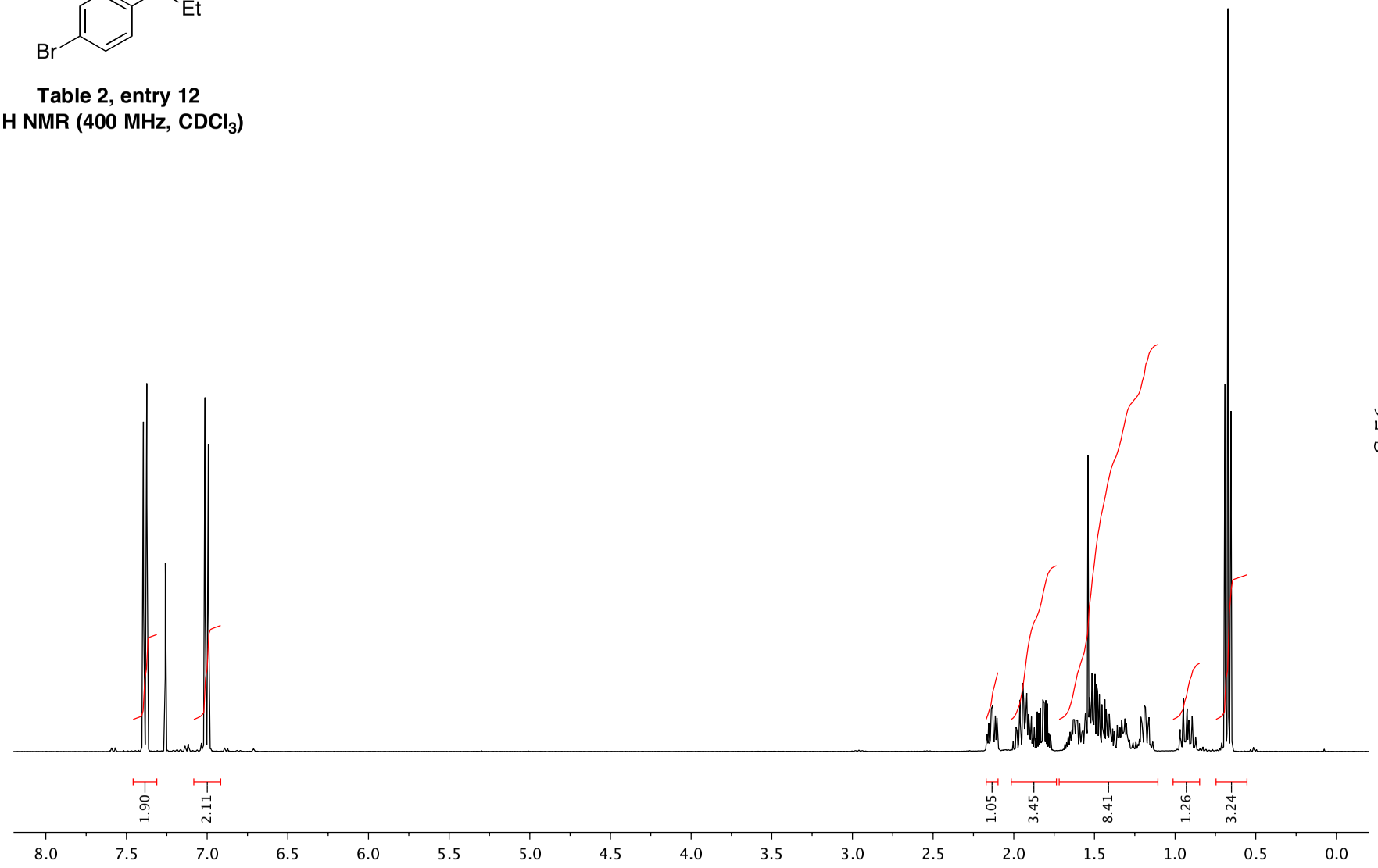


Table 2, entry 12
^{1}H NMR (400 MHz, $CDCl_3$)



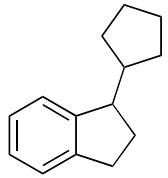
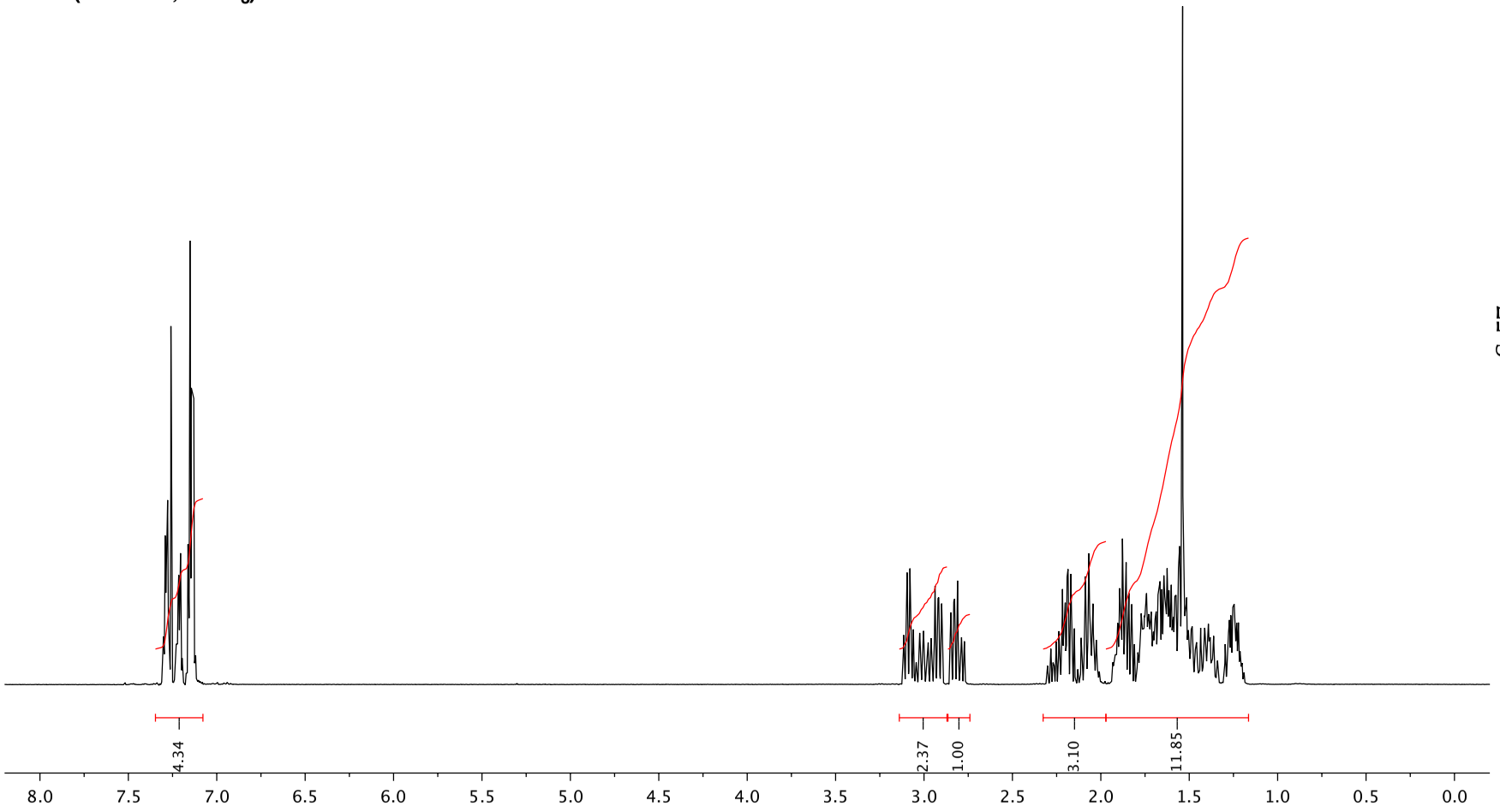


Table 2, entry 13
^{1}H NMR (400 MHz, $CDCl_3$)



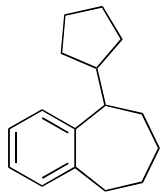
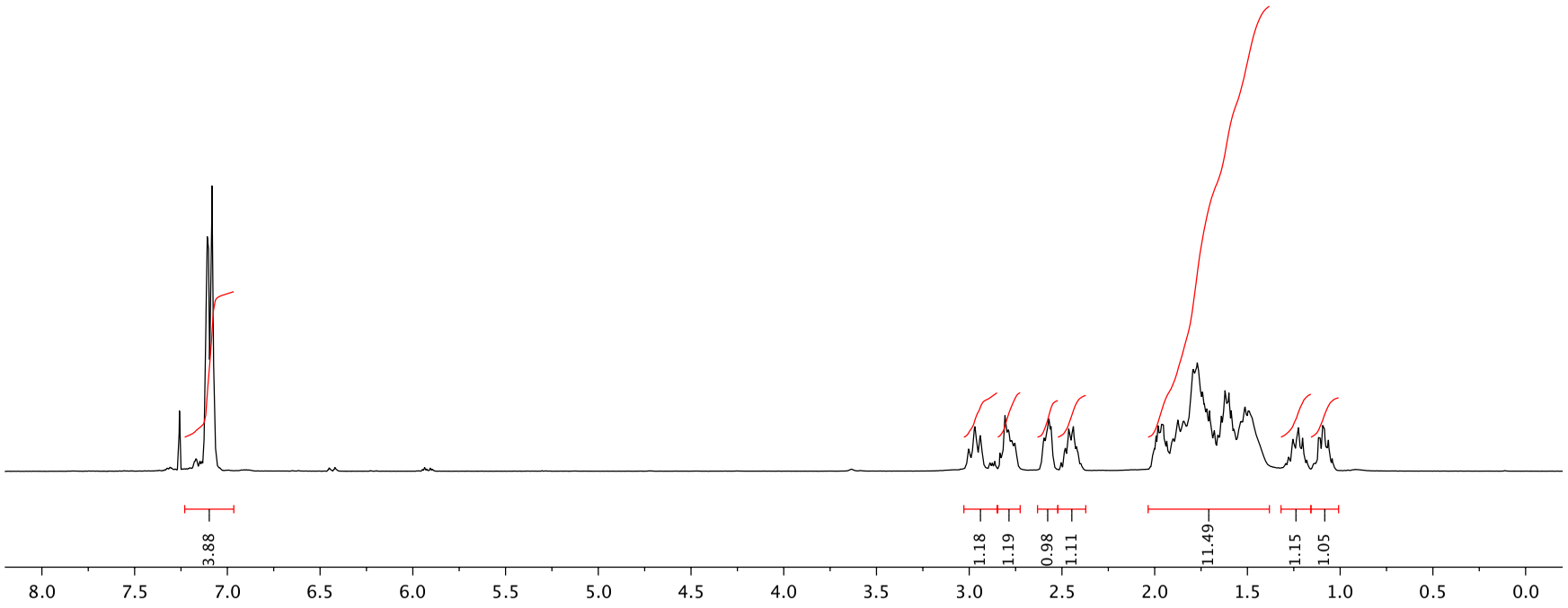


Table 2, entry 14
^{1}H NMR (400 MHz, $CDCl_3$)



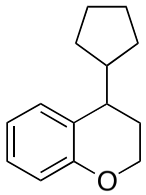


Table 2, entry 15
^{1}H NMR (400 MHz, $CDCl_3$)

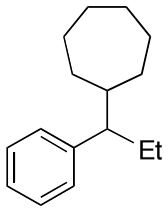
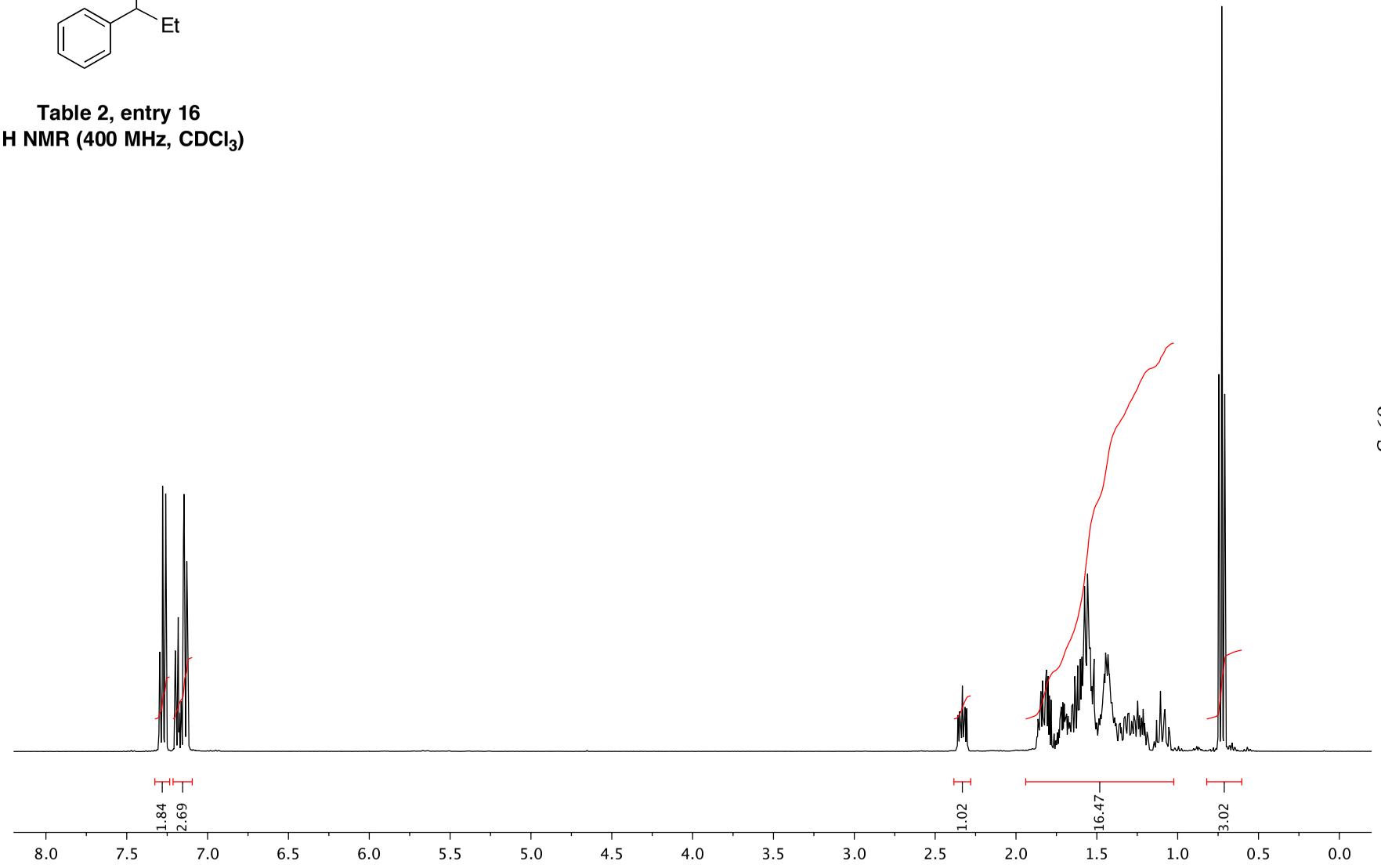


Table 2, entry 16
^{1}H NMR (400 MHz, $CDCl_3$)



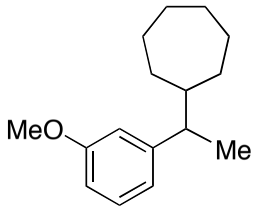
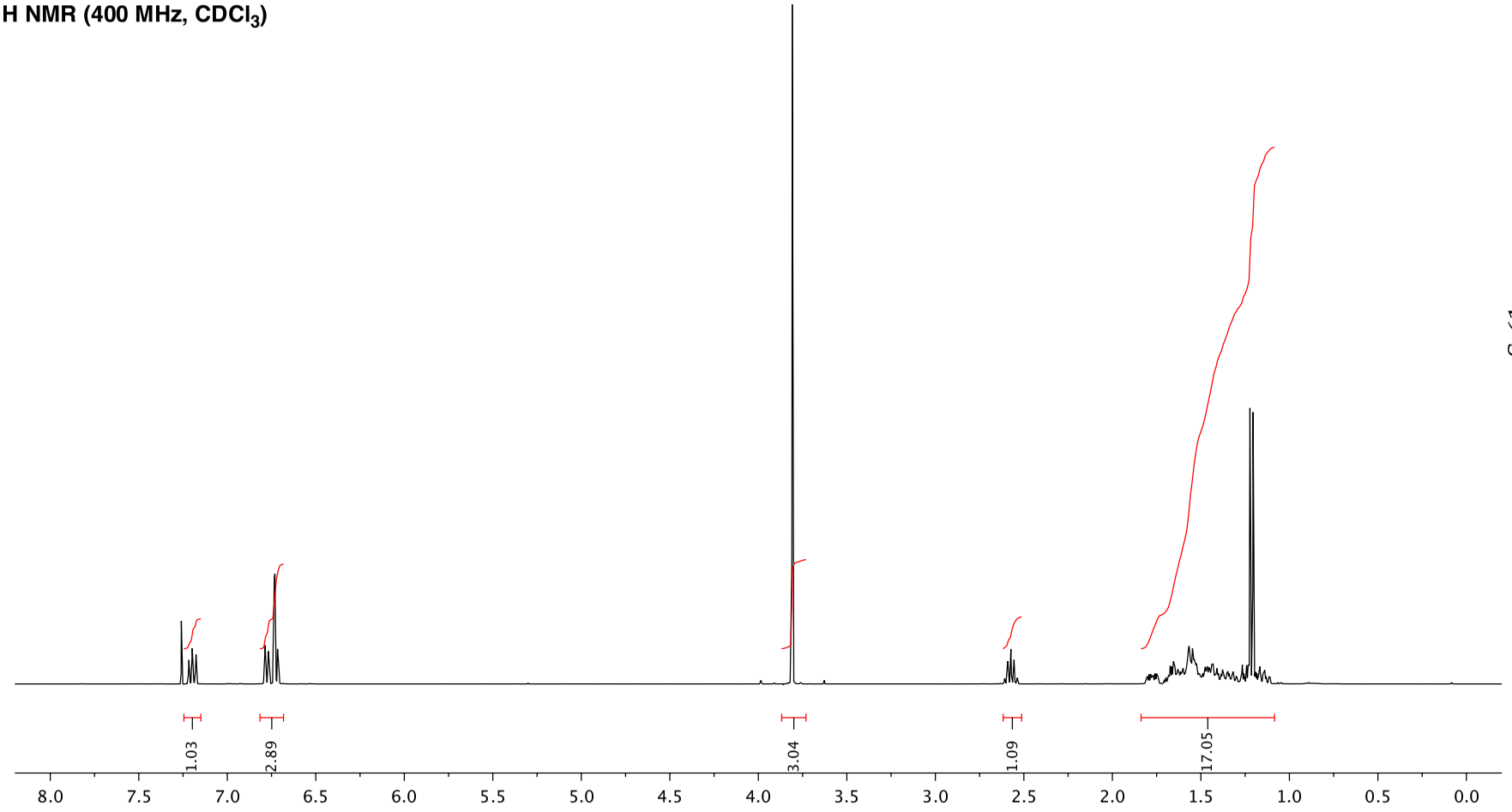
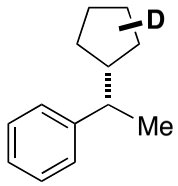
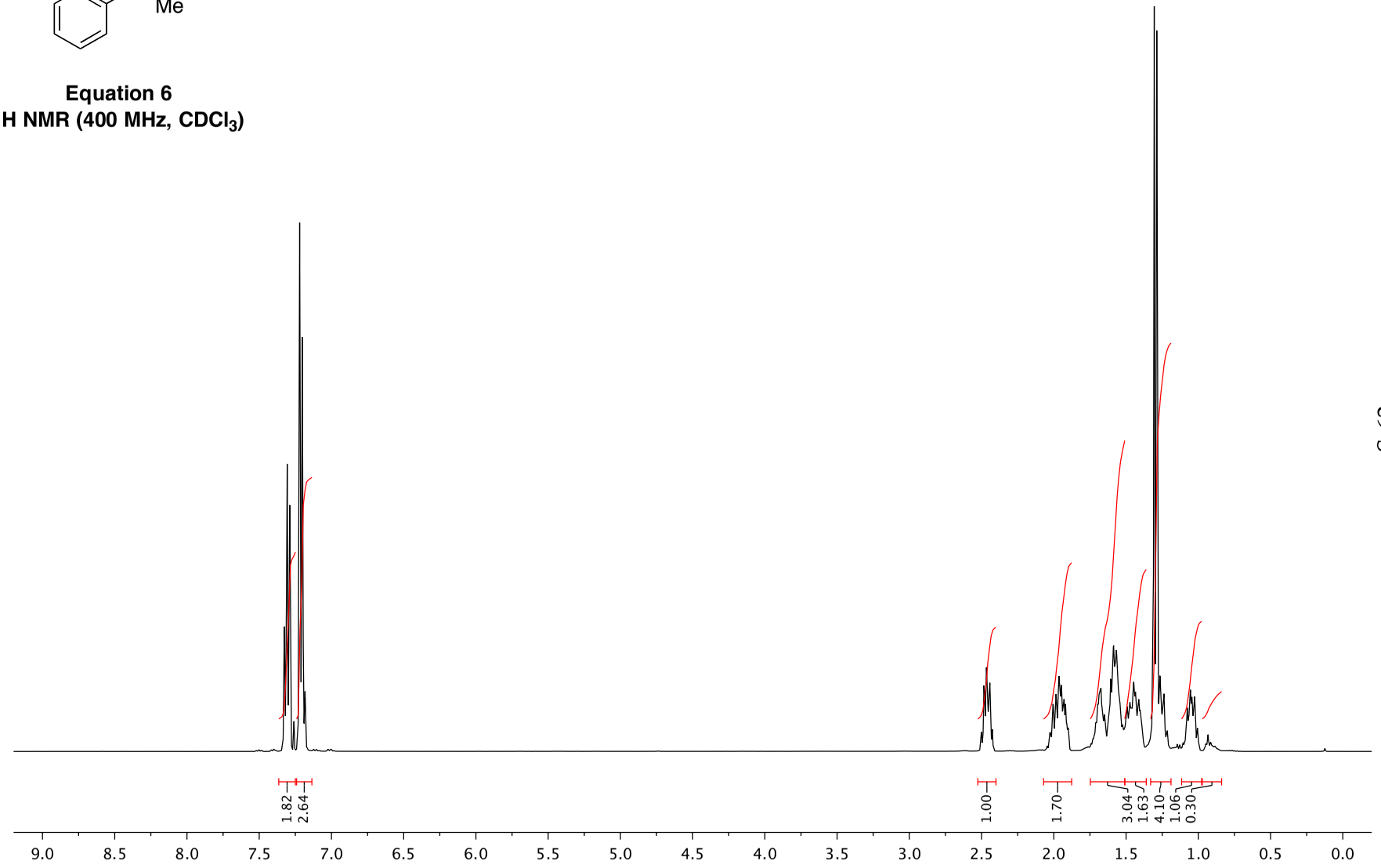


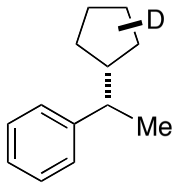
Table 2, entry 17
^{1}H NMR (400 MHz, $CDCl_3$)



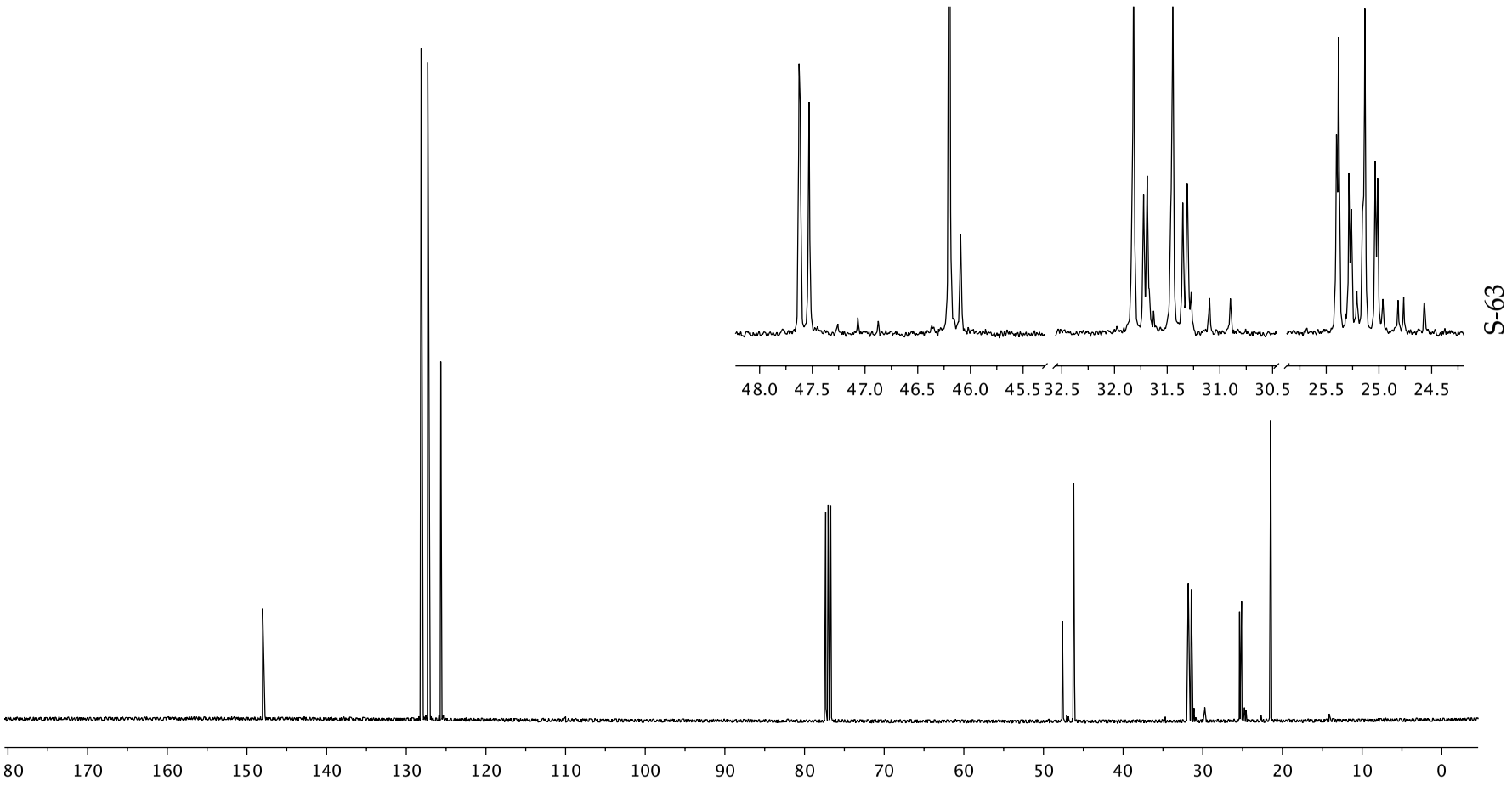


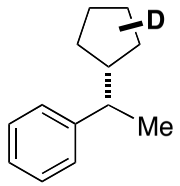
Equation 6
^{1}H NMR (400 MHz, $CDCl_3$)





Equation 6
^{13}C NMR (100 MHz, $CDCl_3$)





Equation 6
$^{13}C\{^{1}H, ^{2}H\}$ NMR (125 MHz, $CDCl_3$)